Fundamental Mechanisms, Predictive Modeling, and Novel Aerospace Applications of Plasma Assisted Combustion

AFOSR
MURI Kick off meeting

The Ohio State University

Nov 4, 2009

Report Documentation Page

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Prescribed by ANSI Std Z39-18

Drexel Group: Main Tasks

Thrust 1. Experimental studies of nonequilibrium air-fuel plasma kinetics using advanced non-intrusive diagnostics

- Task 1: Low-to-Moderate (T=300-800 K) temperature, spatial and time-dependent radical species concentration and temperature measurements in nanosecond pulse plasmas in a variety of fuel-air mixtures pressures (P=0.5-5 atm), and equivalence ratios
- Task 4: Moderate-to-high (T=800 – 1800 K) temperature PAC oxidation kinetics in Discharge Shock Tube Facility at pressures up to 10 bar
- Task 5: PAC oxidation and combustion initiation at high pressure, high temperature conditions

Thrust 2. Kinetic model development and validation

- Task 8: Development and validation of a predictive kinetic model of non-equilibrium plasma fuel oxidation and ignition
- Task 9: Mechanism Reduction and Dynamic Multi-time Scale Modeling of Detailed Plasma-Flame Chemistry

Thrust 3. Experimental and modeling studies of fundamental nonequilibrium discharge processes

- Task 10: Characterization and Modeling of Nsec Pulsed Plasma Discharges

Thrust 4. Studies of diffusion and transport of active species in representative two-dimensional reacting flow geometries

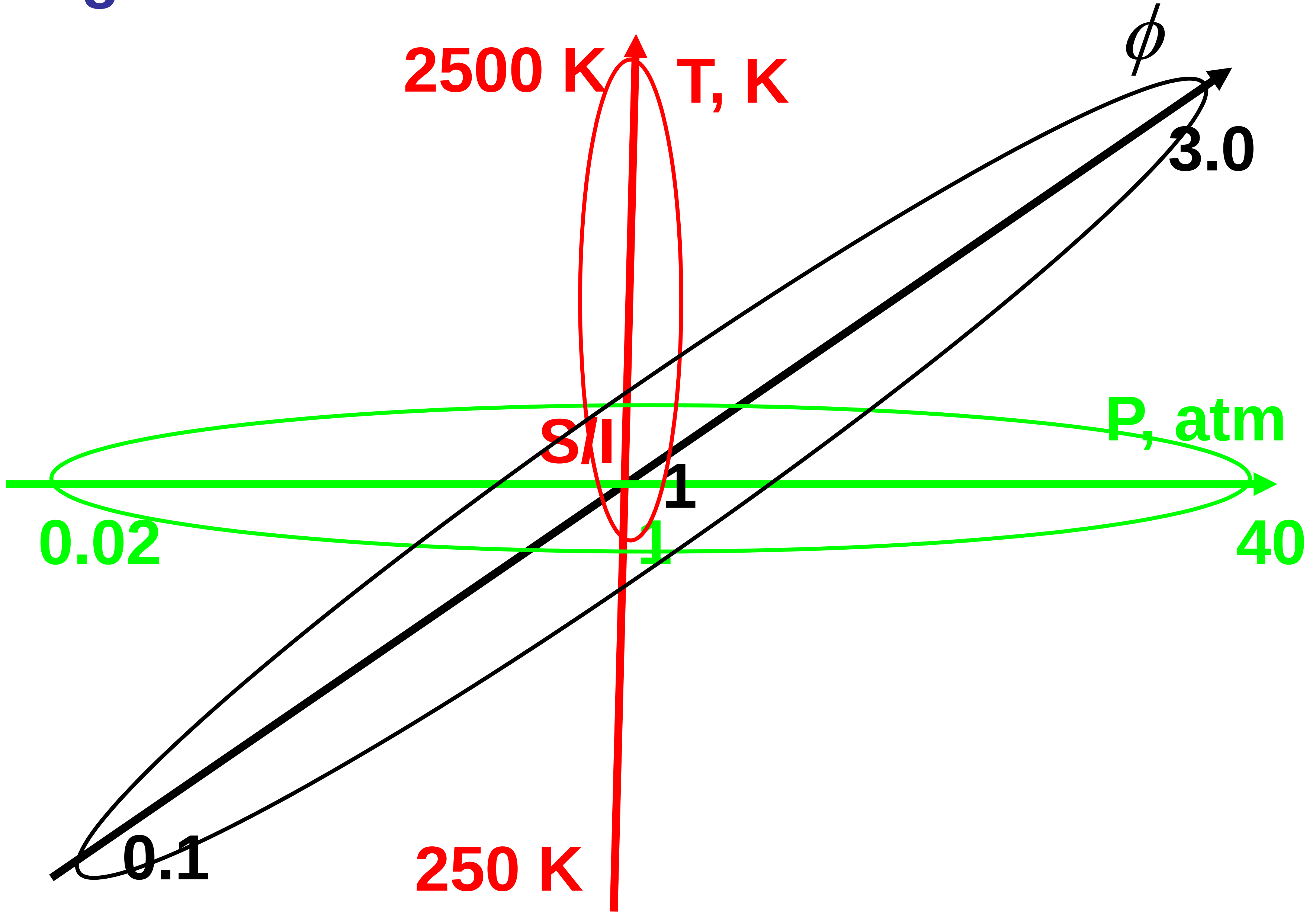
- Task 13: Ignition and flameholding in high-speed non-premixed flows
- Task 14: High Fidelity Modeling of Plasma Assisted Combustion in Complex Flow Environments

Drexel Group: International Collaboration

International Collaborators

Svetlana Starikovskaya (Ecole Pol)	– Thrust 1
Alexander Rakitin (NEQLab)	– Thrust 1
Boris Potapkin (KIAE)	– Thrust 2
Alexander Konnov (VUB)	– Thrust 2
Nickolay Aleksandrov (MIPT)	– Thrust 3
Sergey Pancheshnyi (Univ Toulouse)	– Thrust 3
Sergey Leonov (IVTAN)	– Thrust 4

Range of Parameters – Combustion Kinetics



Problems of Plasma-Chemical Models

Availability and accuracy of data on electron collision cross sections

+ H_2 CH_4 C_2H_6 C_3H_8

? C_4H_{10} C_5H_{12} …

Availability and accuracy of chemical models below self-ignition point

+ H_2

? CH_4 C_2H_6 C_3H_8 C_4H_{10} C_5H_{12} …

Availability and accuracy of physical and chemical models for non-equilibrium conditions

+ Radical’s mechanism

? Ionic chain mechanism

? Energy chain mechanism

Models for Low-Temperature Plasma Assisted Combustion

Starikovskii et al.,

Plasma Physics Reports, 2000 (26) 701

$O_2 + e^- + M \rightarrow O_2^- + M$

$H_2 + O_2^- \rightarrow OH^- + OH$

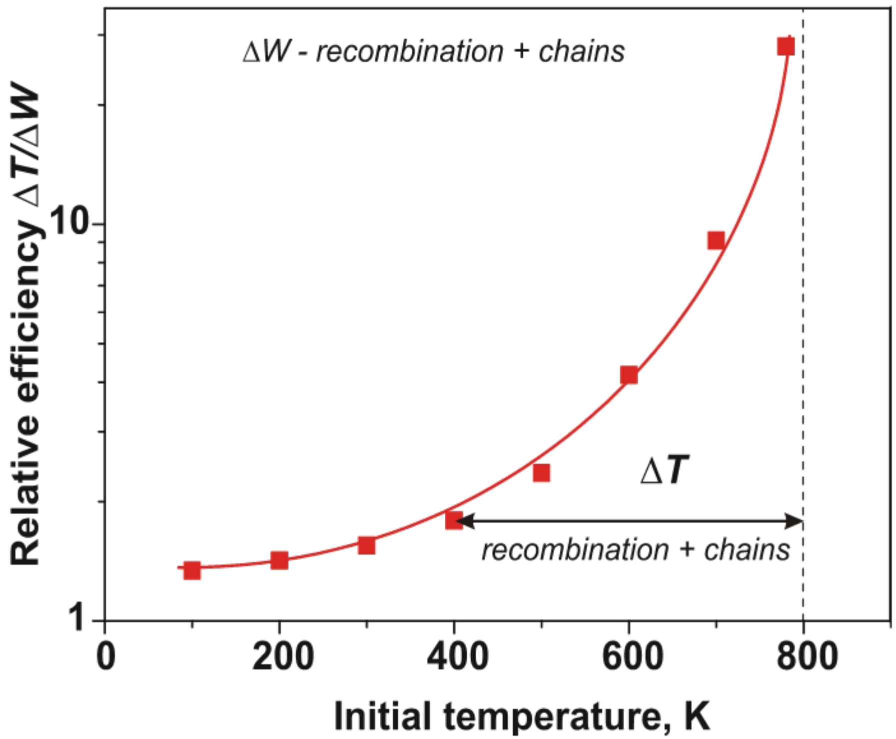
$OH + H_2 \rightarrow H_2O + H$

$OH^- + H \rightarrow H_2O + e^-$

$H + O_2 + M \rightarrow HO_2 + M$

$OH^- + HO_2 \rightarrow H_2O + O_2 + e^-$

800 K: autoignition gives 1 s



Starikovskii,

Chemical Physics Reports, 2003 (11) 1

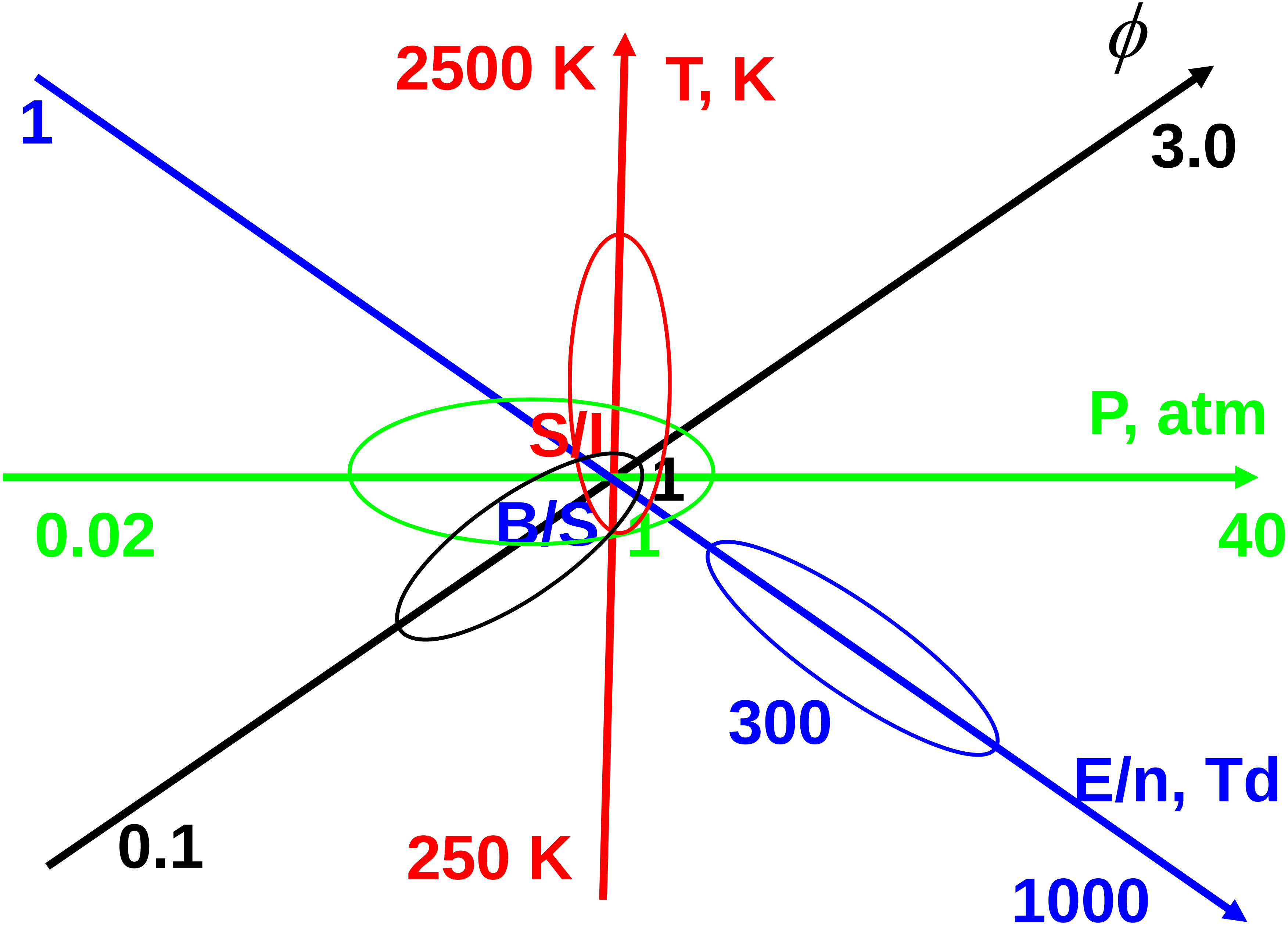
$N_2O^* + H \rightarrow N_2^* + OH$

$CO + OH \rightarrow CO_2^* + H$

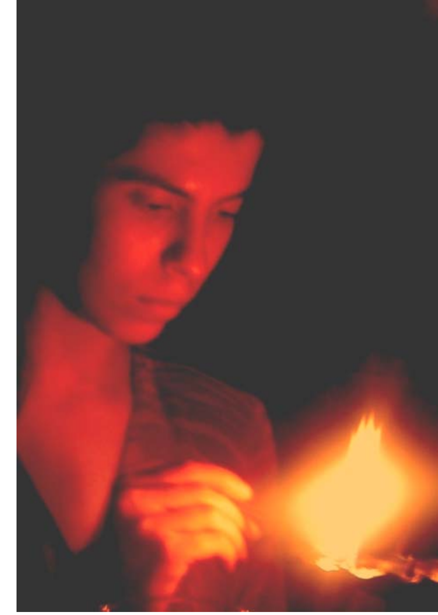
$CO_2^* + N_2O \rightarrow N_2O^* + CO_2$

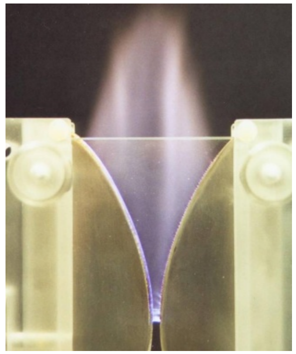
$N_2^* + N_2O \rightarrow N_2O^* + N_2$

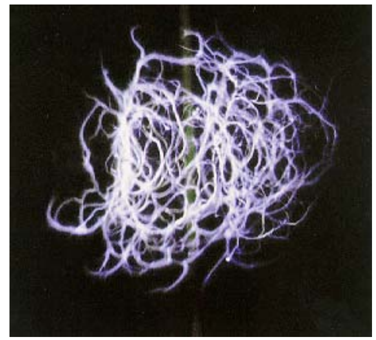
PAC: Where we are



Mechanisms of Plasma Influence

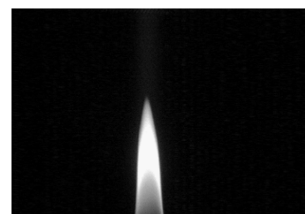




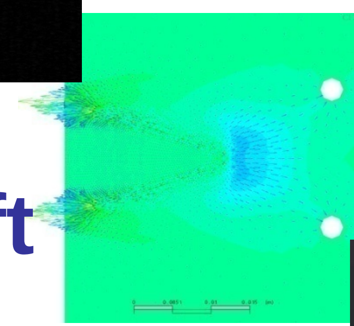


1. Heating

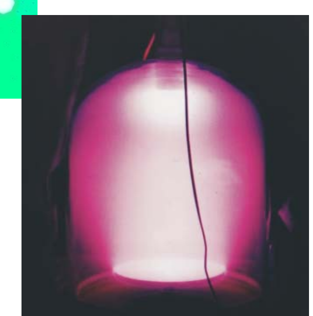
2. Turbulization



3. Momentum Transfer

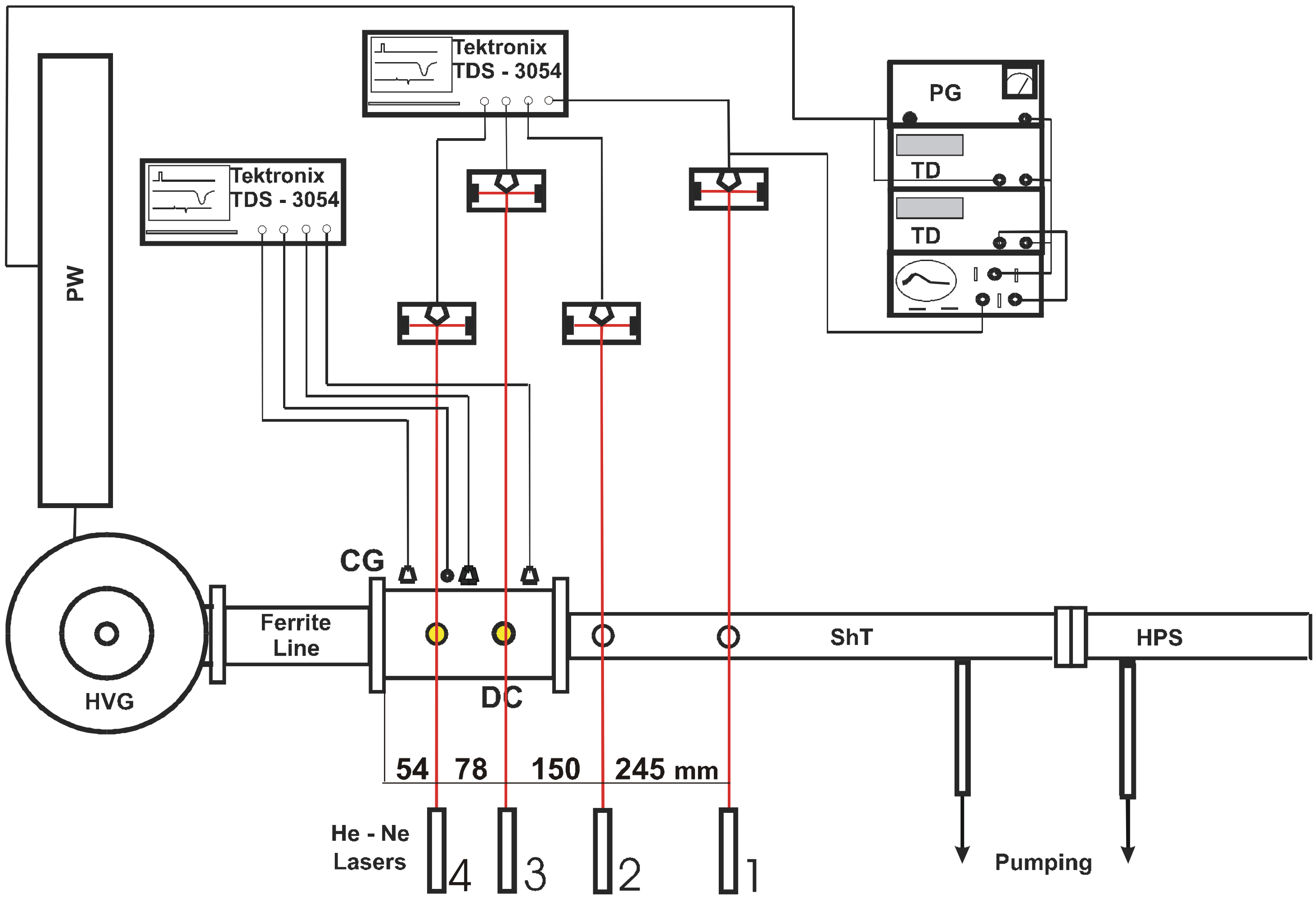


4. Electrons/Ions Diffusion/Drift

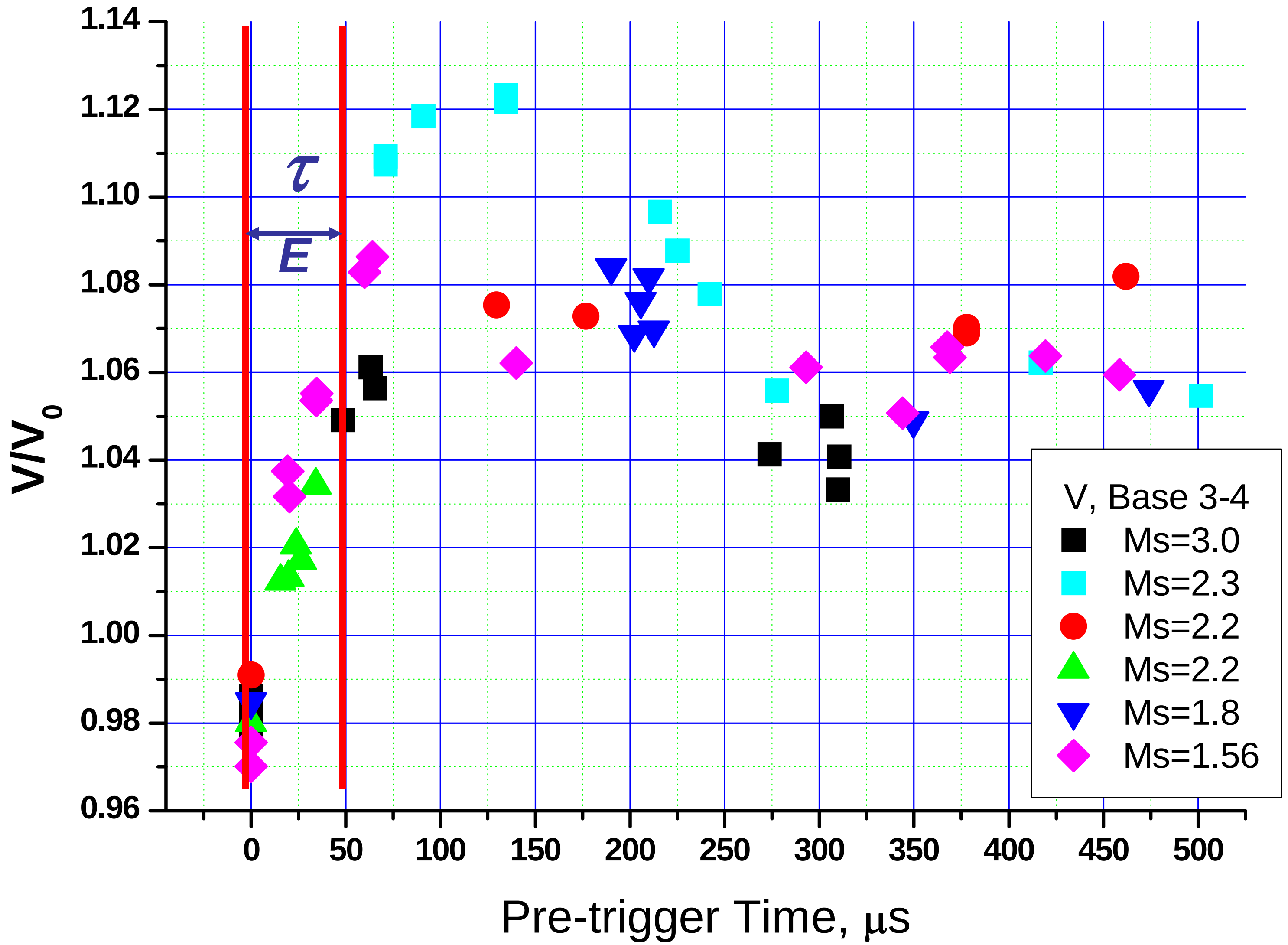


5. Dissociation, Ionization

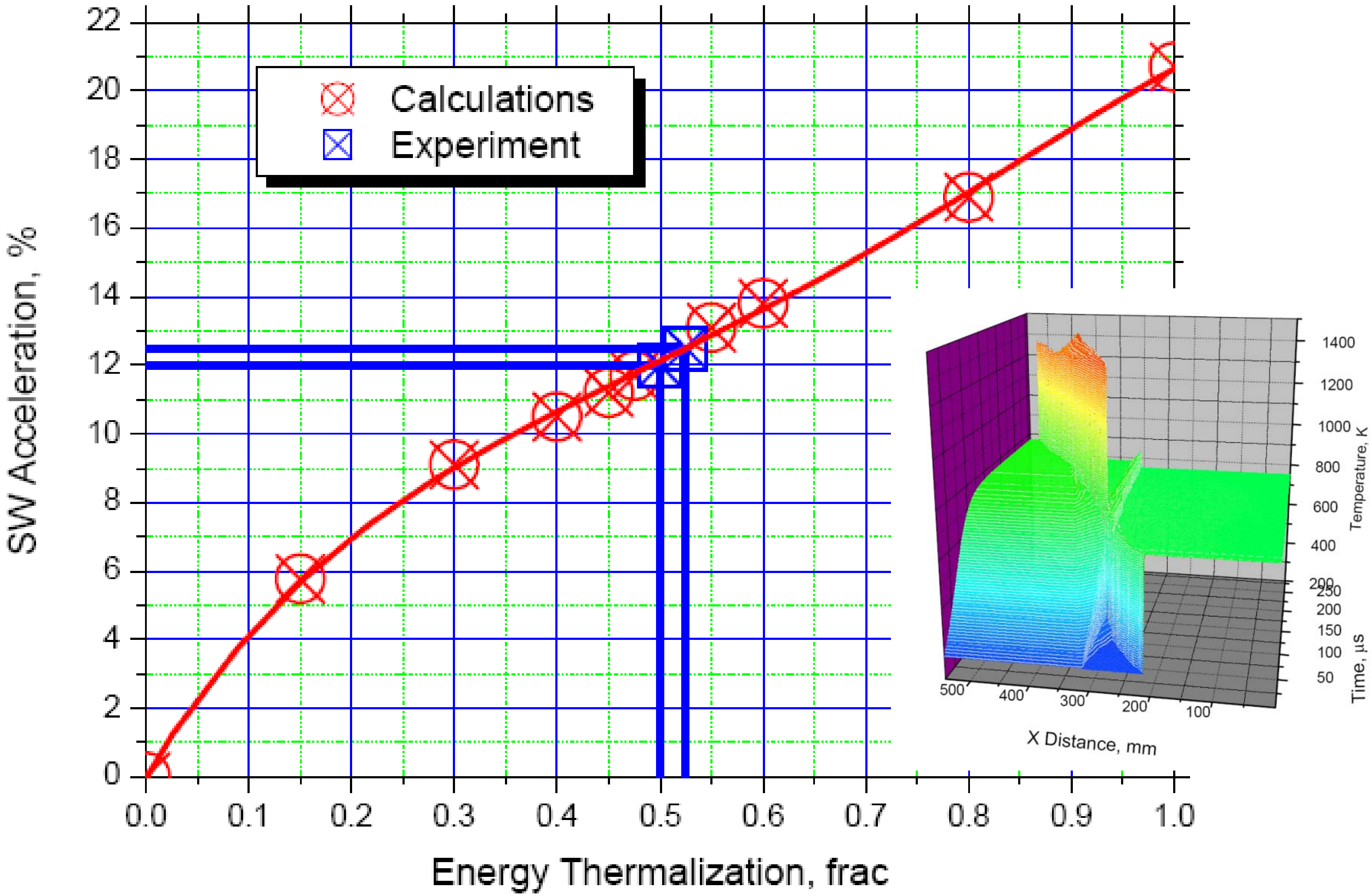
Shock Wave - Nonequilibrium Plasma Interaction



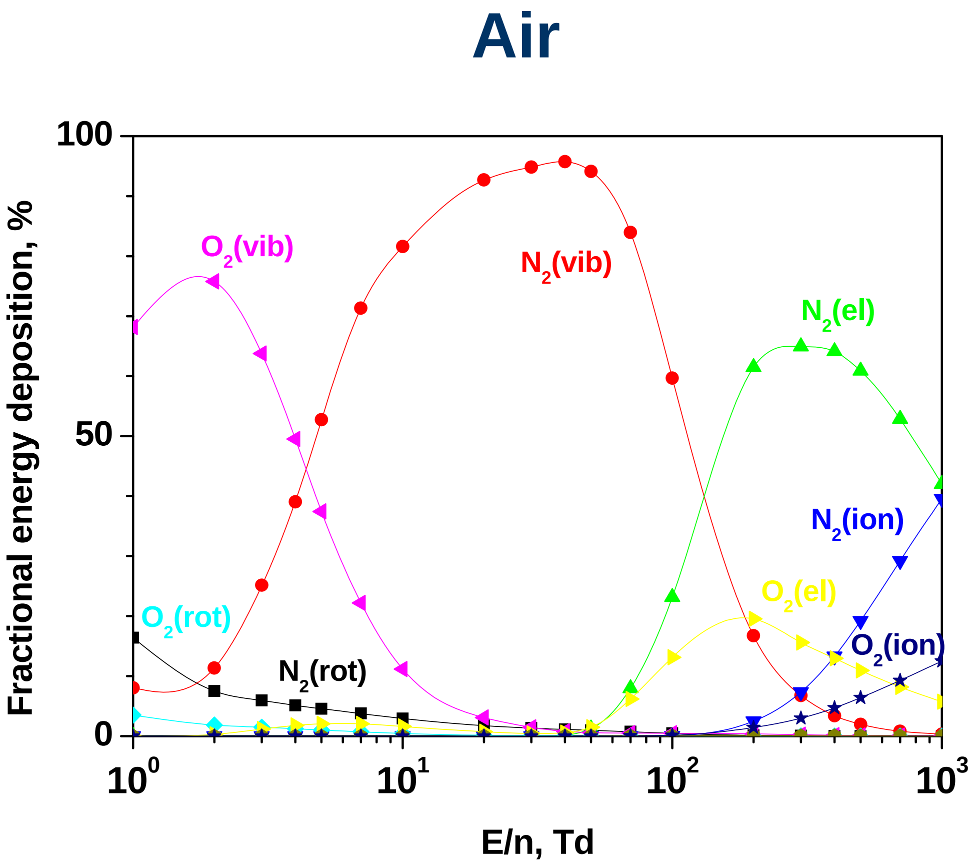
Relaxation of Nonequilibrium Plasma.
Air. P_1 ~ 20 Torr



Relaxation of Nonequilibrium Plasma.
Air. P_1 ~ 20 Torr



Mechanism of fast heating in discharge plasmas (low E/N)



Low (< 20 Td) E/N:

e + N_2 , O_2

- elastic scattering

- rotational excitation

Mechanism of fast heating in discharges (moderate E/N)

Moderate (20 - 200 Td) E/N:

Popov (2001) heating $\rightarrow$ 28 % of power spent on $N_2^* + O_2^*$

$e + O_2 \rightarrow e + 2O + \Delta E$

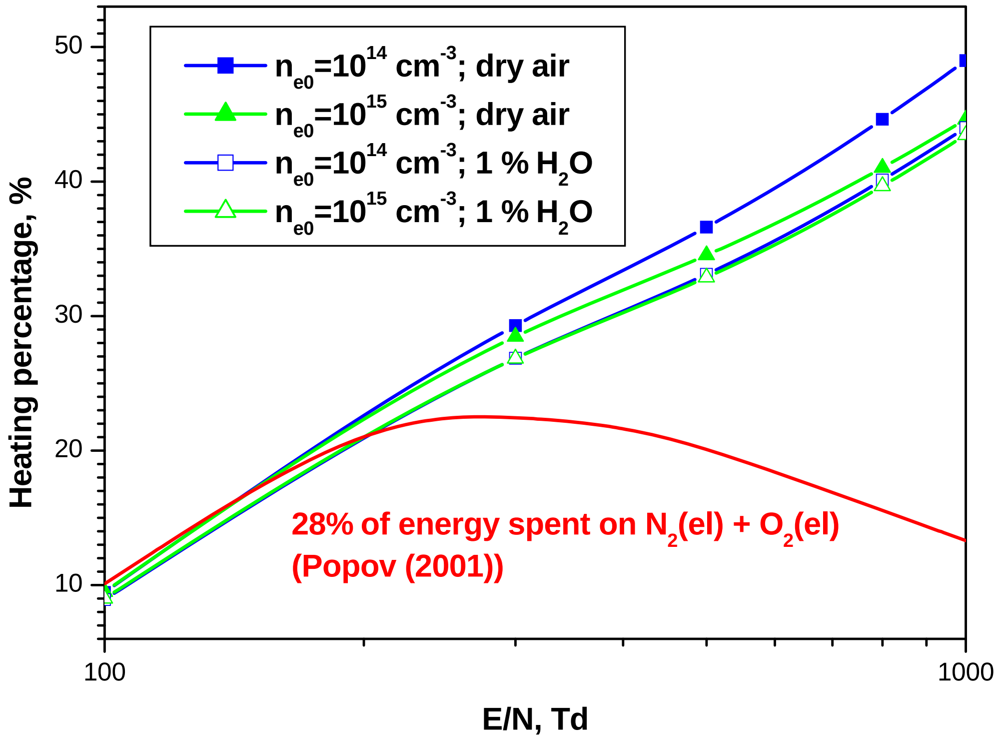
$e + N_2 \rightarrow e + N_2^*(A, B, C, a', ...)$

$N_2^*(A, B, C, a', ...) + O_2 \rightarrow N_2 + 2O + \Delta E$

$O(^1D) + N_2 \rightarrow O + N_2 + \Delta E$ $k \sim 10^{-10}\ cm^3/s$

Mechanism of fast heating in discharge plasmas (high E/N)

Aleksandrov et al. (2009)



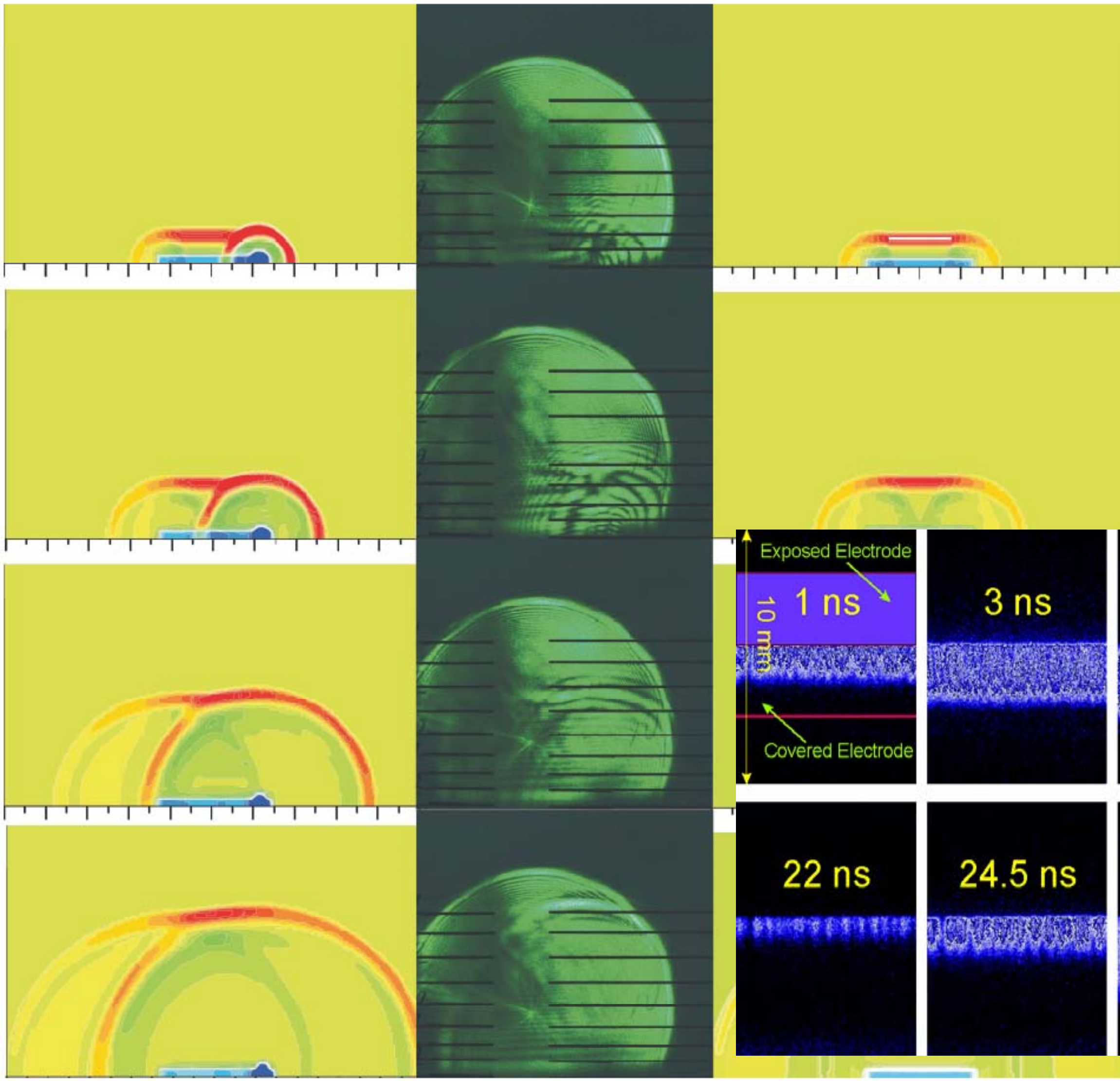
High (> 200 Td) E/N:

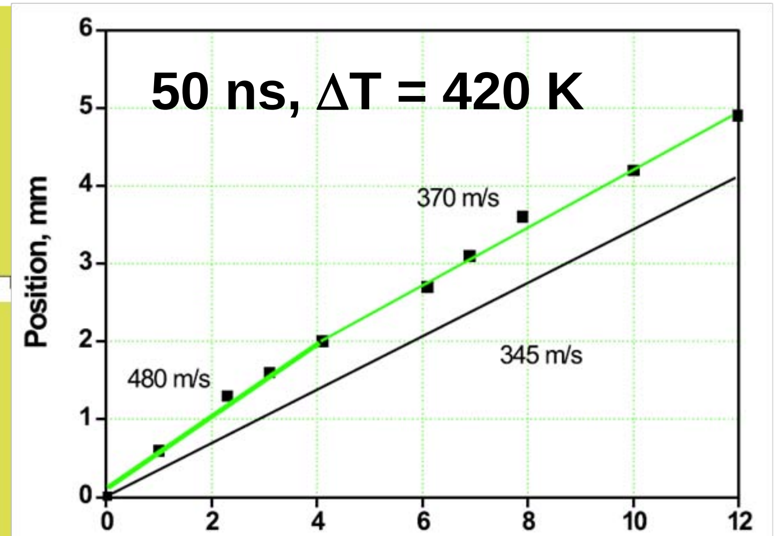
electron-ion and ion-ion recombination kinetics

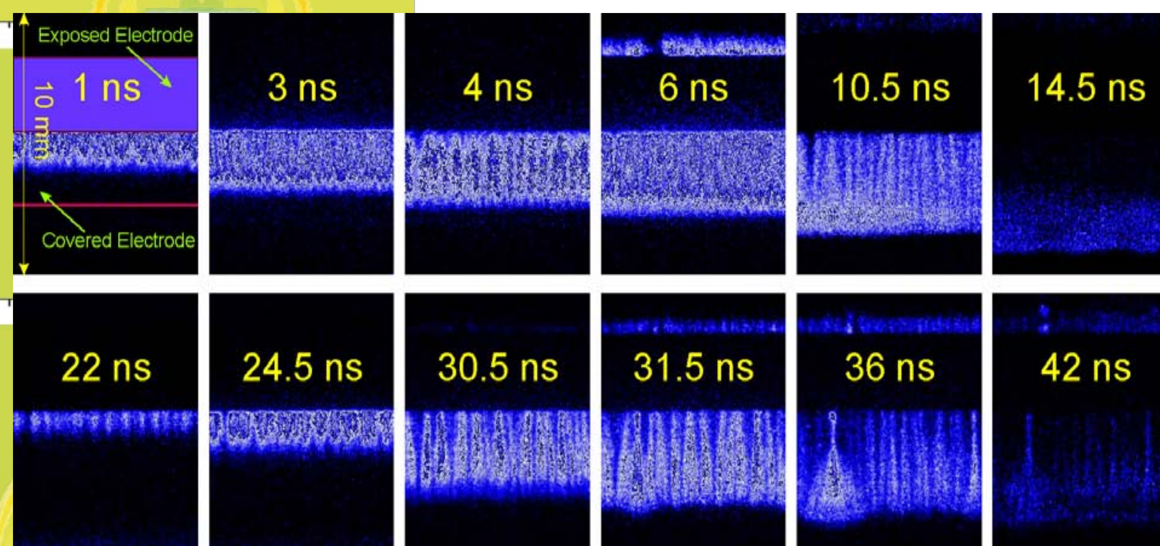
$$e + O_2^+ \rightarrow O + O^* + \Delta E$$

$$O_2^- + O_2^+ + M \rightarrow 2O_2 + M + \Delta E$$

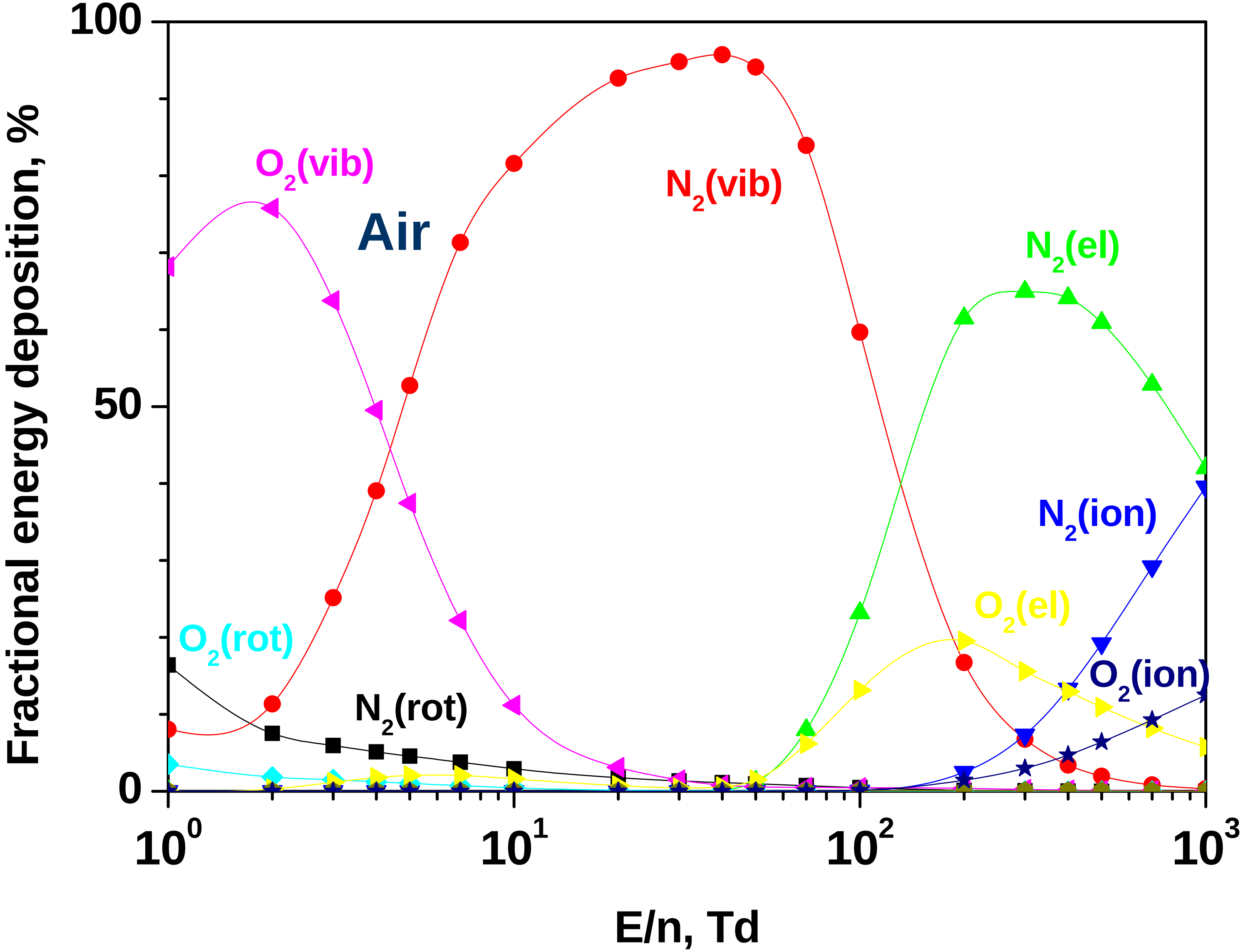
Heat Release and Shock Waves Formation by "Nonequilibrium" Plasma







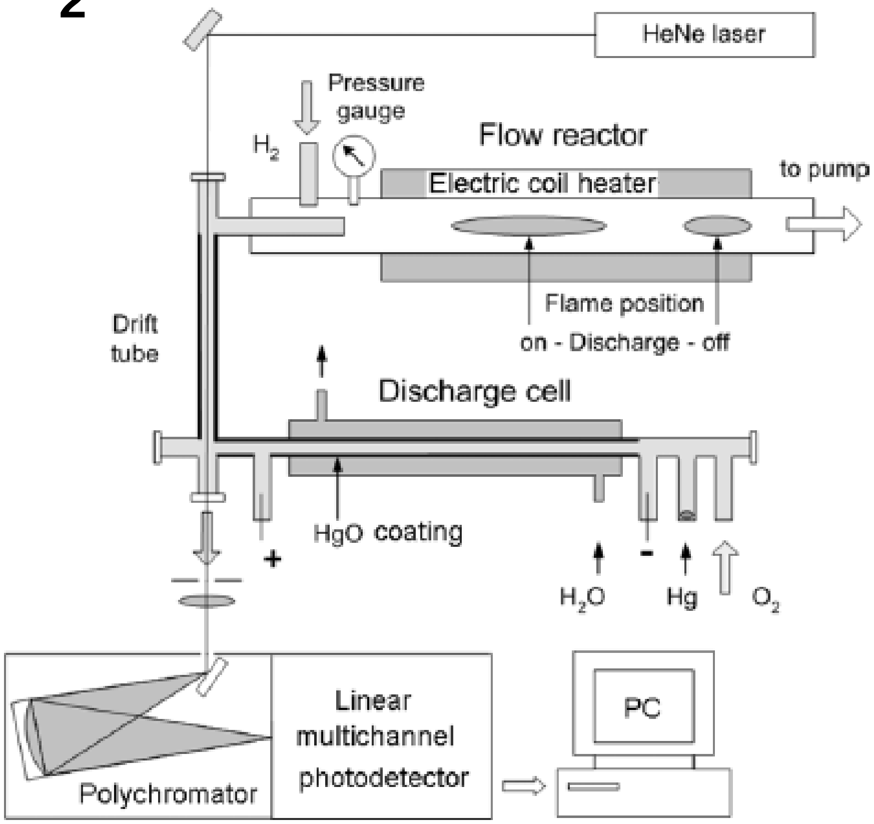
Energy Distribution in Gas Discharge



Molecular Oxygen Excitation

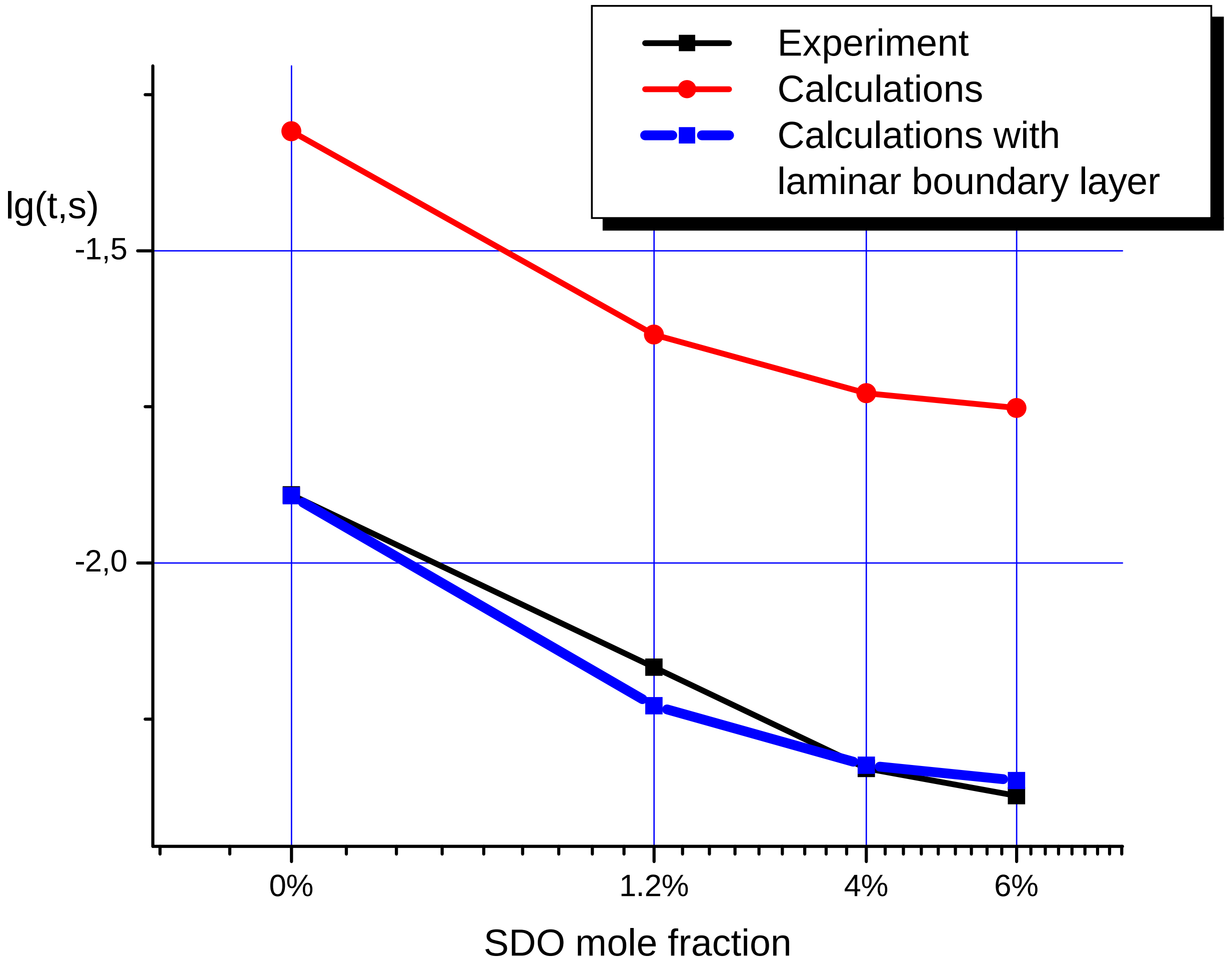
To directly observe the influence of SDO on the combustion of H_2-O_2 mixture

- **Delivering sufficient amount of SDO**
- **Minimizing the effect of O atom**
- **Lower the inlet temperature**



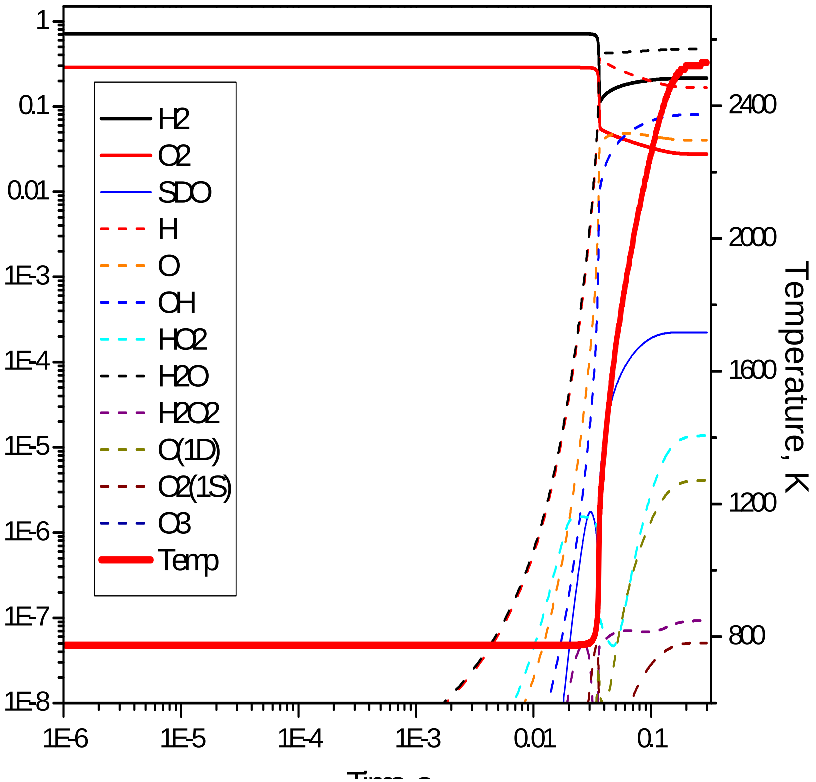
V V Smirnov, O M Stelmakh, V I Fabelinsky, D N Kozlov, A M Starik and N S Titova, *J. Phys. D: Appl. Phys*. 41 (2008)

SDO kinetic analysis



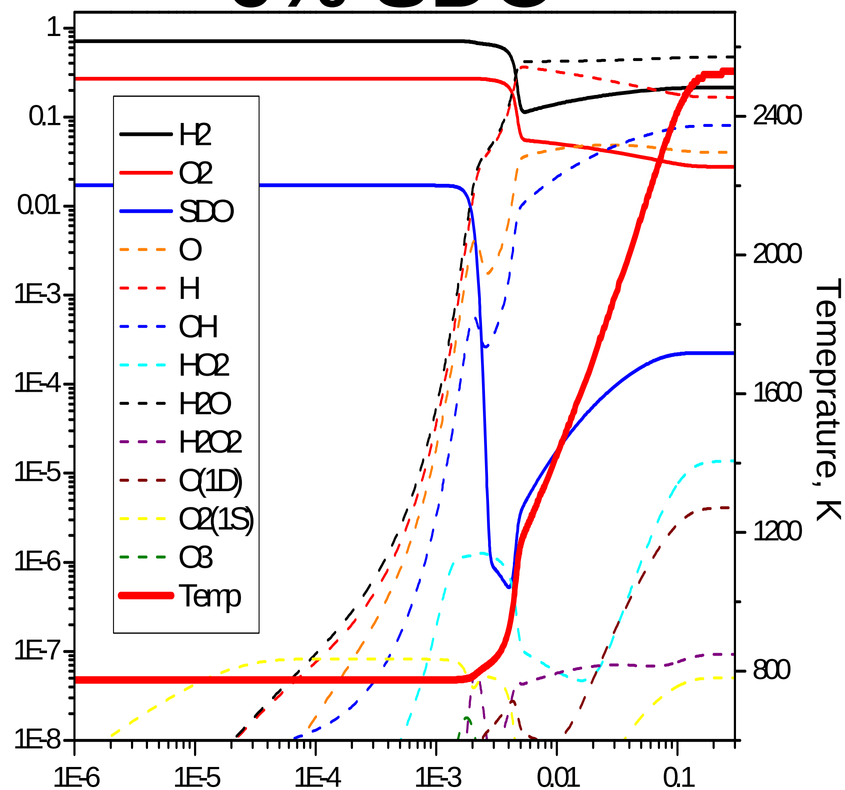
The ignition time as a function of SDO mole fraction in oxygen.
T=775 K and P=10 Torr in the H_2:O_2=5:2 mixture

SDO kinetic analysis



Auto-ignition

6% SDO



The evolution in time of the mole fractions of the main component for autoignition (a) and ignition with 6% singlet delta oxygen. The gas temperature evolution is represented by the thick red line.

SDO kinetic analysis

Possible reasons

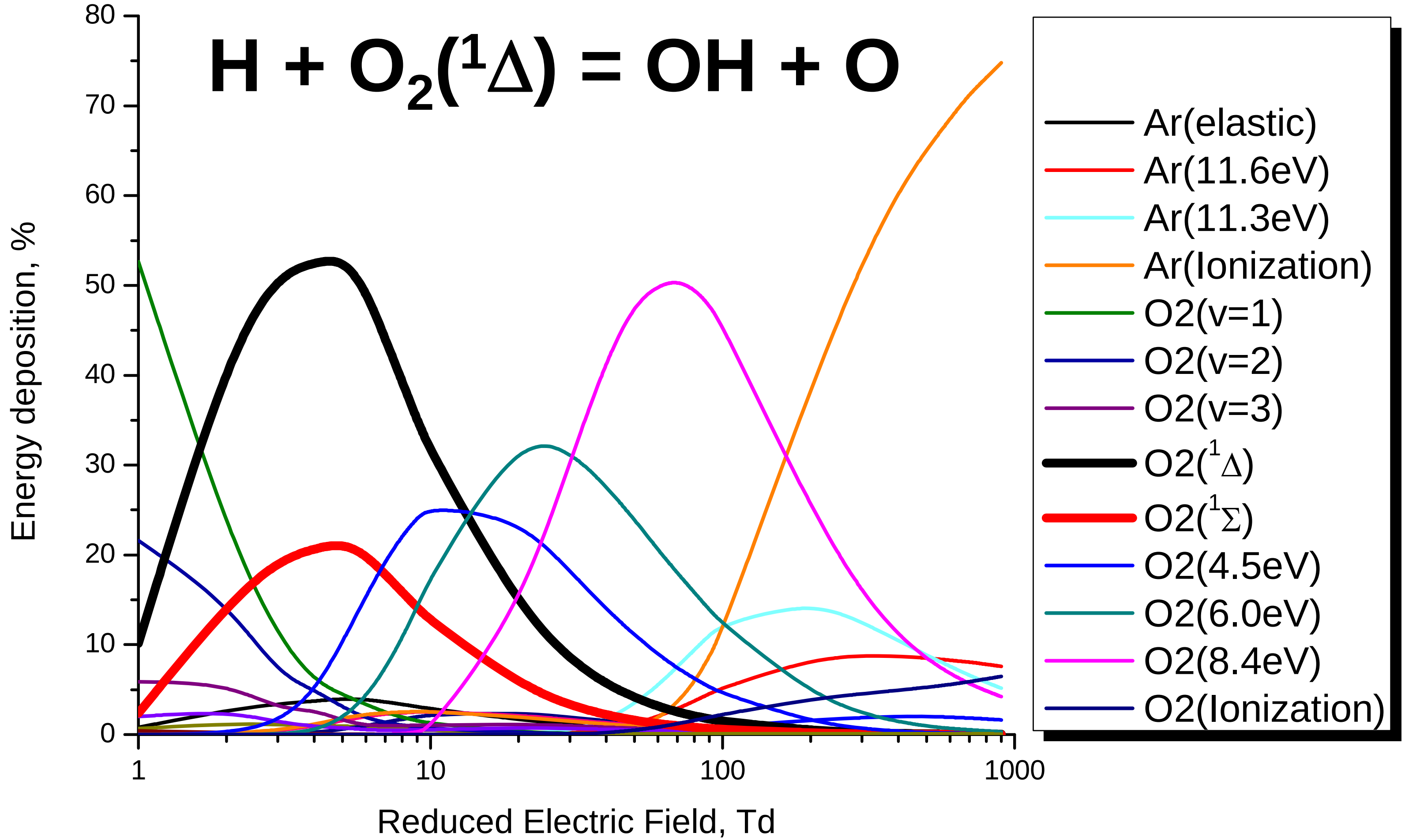
Auto	SDO
$O_2+M=O+O+M$ (slow) $H_2+O=OH+H$ $O_2+H=OH+O$ $OH+OH=H_2O+O$ … …	$O_2(a^1\Delta_g)+H_2=OH+OH$ (fast) $OH+H_2=H_2O+H$ $O_2(a^1\Delta_g)+H=OH+O$ $O_2+H=OH+O$ $OH+OH=H_2O+O$ …

Radical generation efficiency

$\boxed{O_2(a^1\Delta_g)+H_2=OH+OH}$ $\xrightarrow[\sim 80\ \mu s]{}$ $\boxed{O_2(a^1\Delta_g)+H=OH+O}$

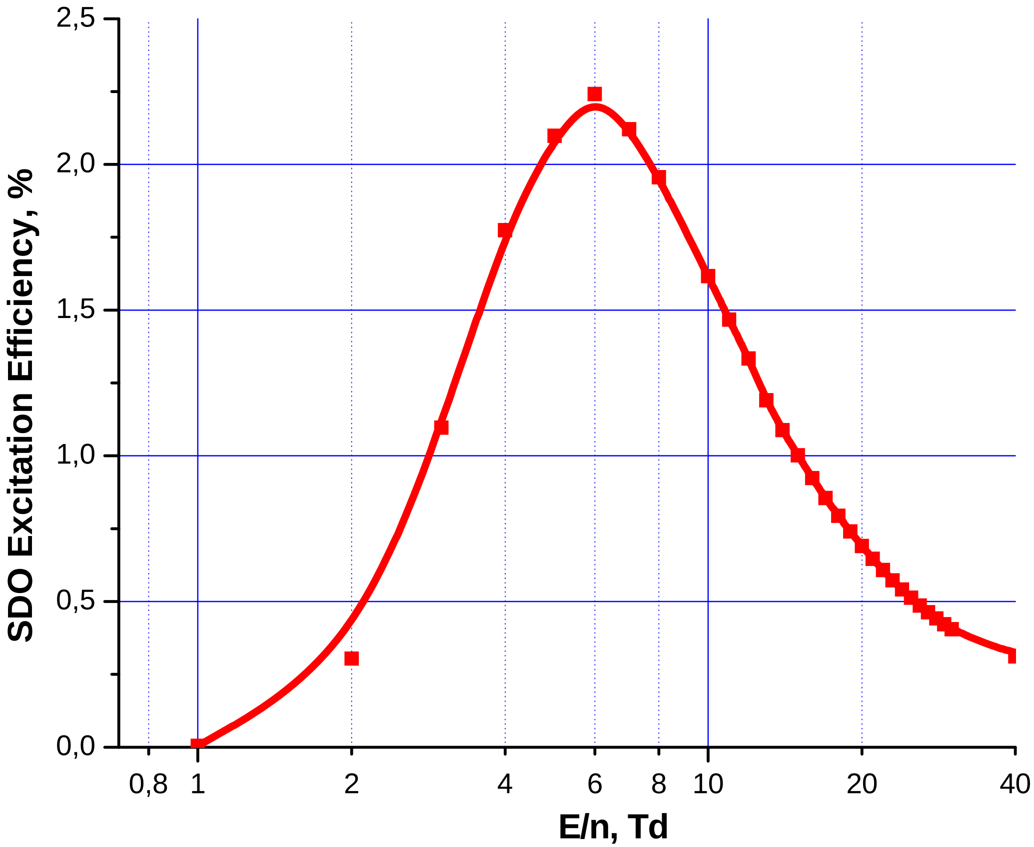
200% 100%

Energy Distribution in O_2-Ar (15%:85%) Mixture



- **74% energy in excitation of singlet oxygen at E/n= 5 Td**
  - **Approximately 53% in singlet delta state**
    - **About 21% in singlet sigma state**

SDO Excitation efficiency in air plasma



Air Plasma

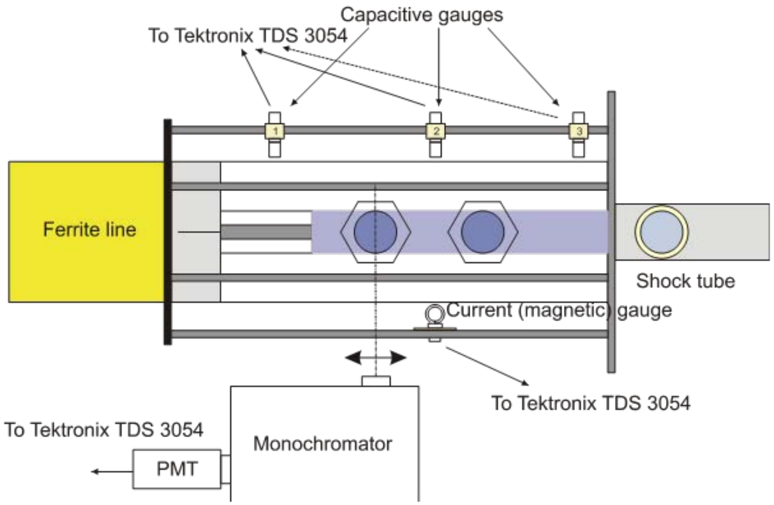
E/n = 6 Td (=10^{-17} Vcm^2)

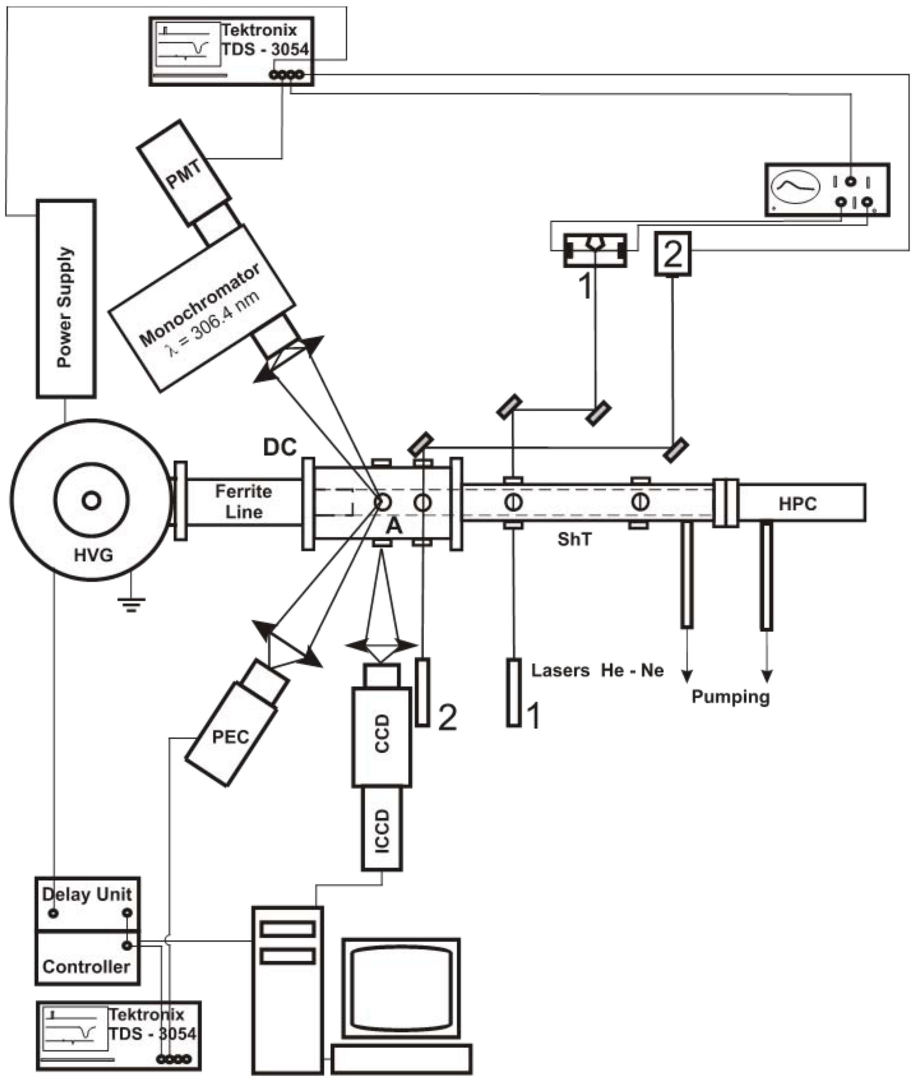
N2 Elastique	1.8 %
N2(ROT)	4 %
N2 (V=1)	49 %
N2 (V=2)	7.3 %
N2 (V=3)	1.4 %
N2 (V=4)	0.2 %
O2 Elastique	0.3 %
O2 (ROT)	0.2 %
O2 (V=1)	17 %
O2 (V=2)	11 %
O2 (V=3)	4.1 %
O2 (V=4)	1.4 %
O2 ($a^1\Delta_g$)	2.2 %
O2 ($b^1\Sigma$)	0.1%

Shock Tube with Discharge Section.
U ≤ 0.3 MV, M ≤ 3

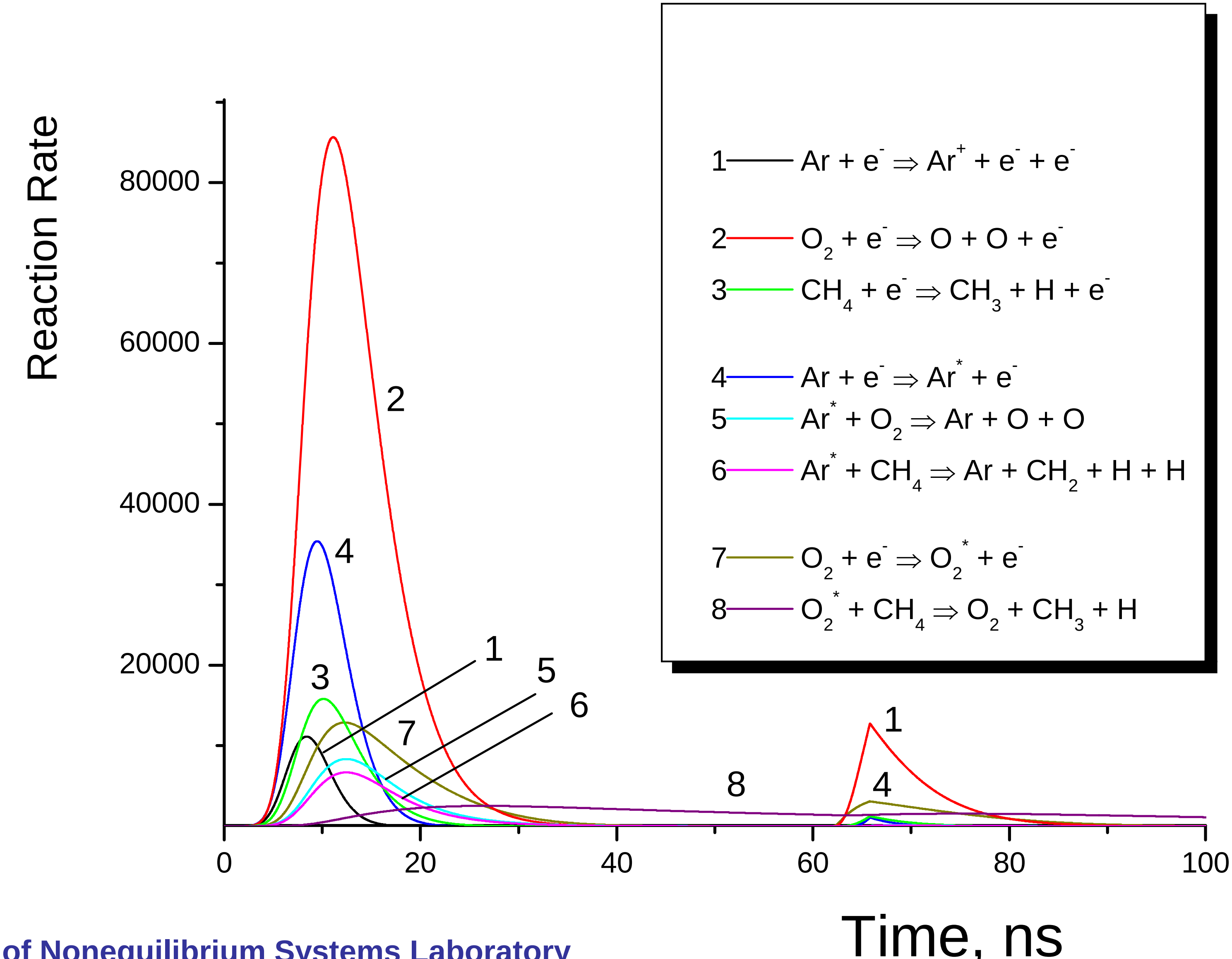
Starikovskaya et al

Test Section of the Shock Tube

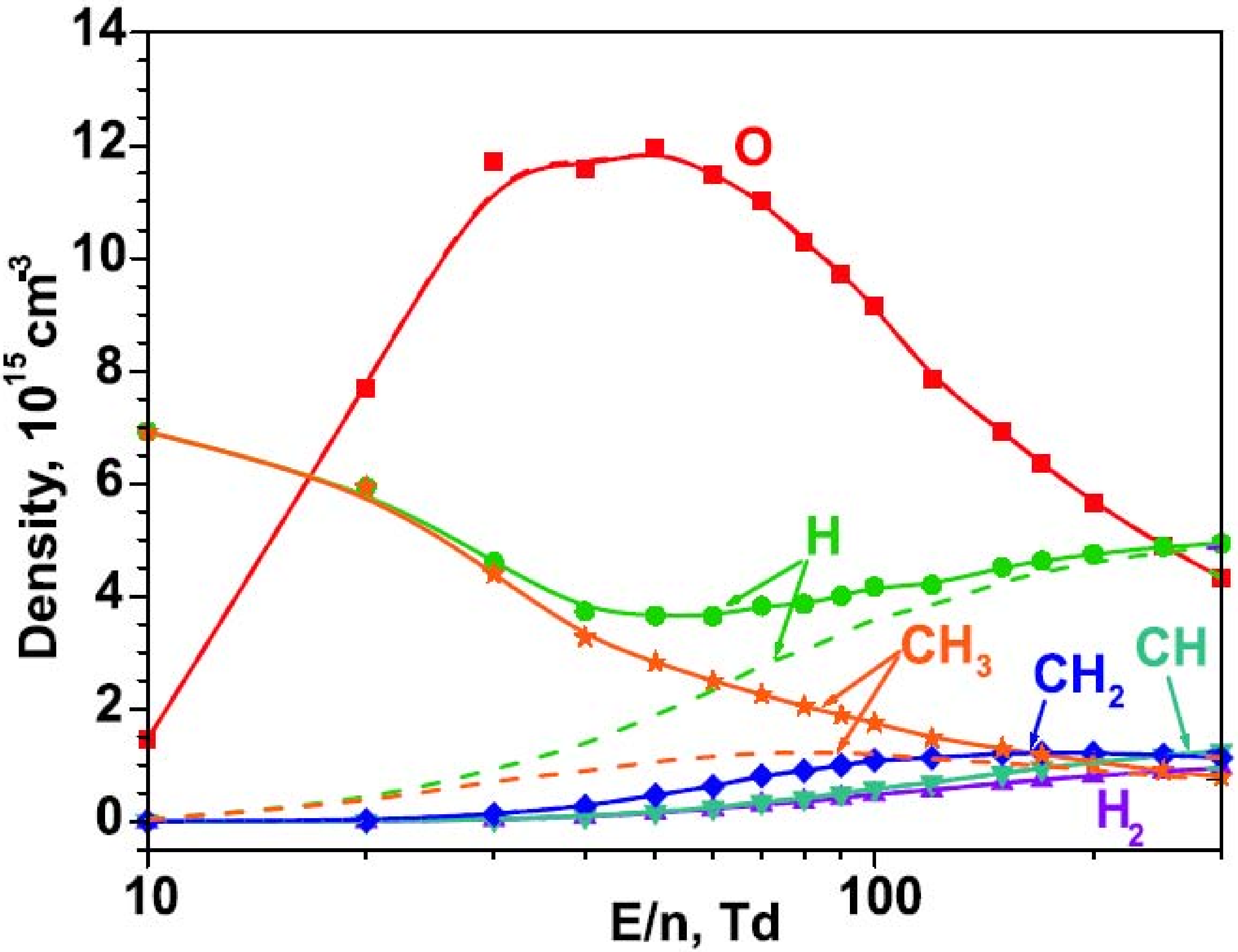




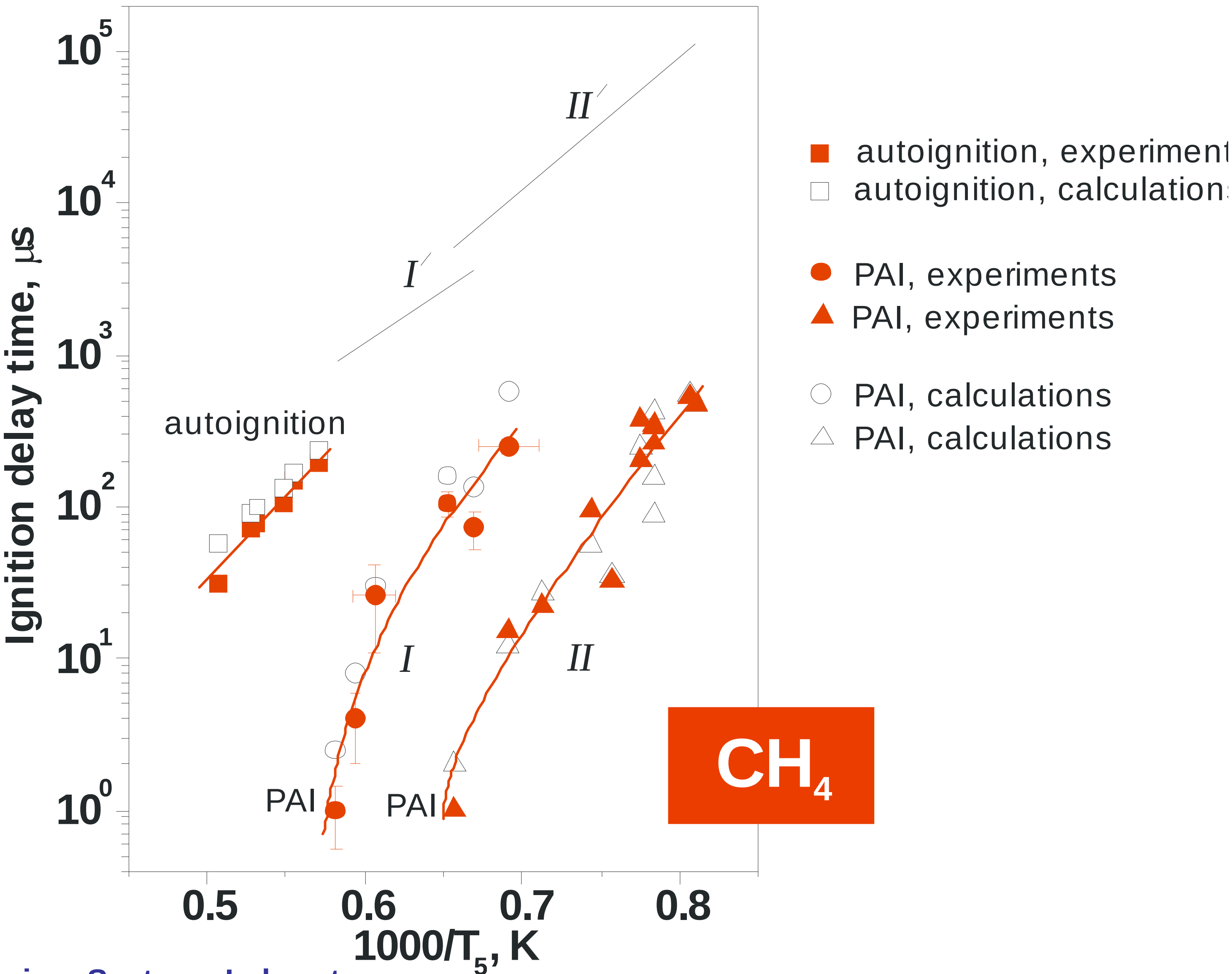
Main Processes During Discharge Phase



Radicals Production in Discharge CH_4-containing mixture

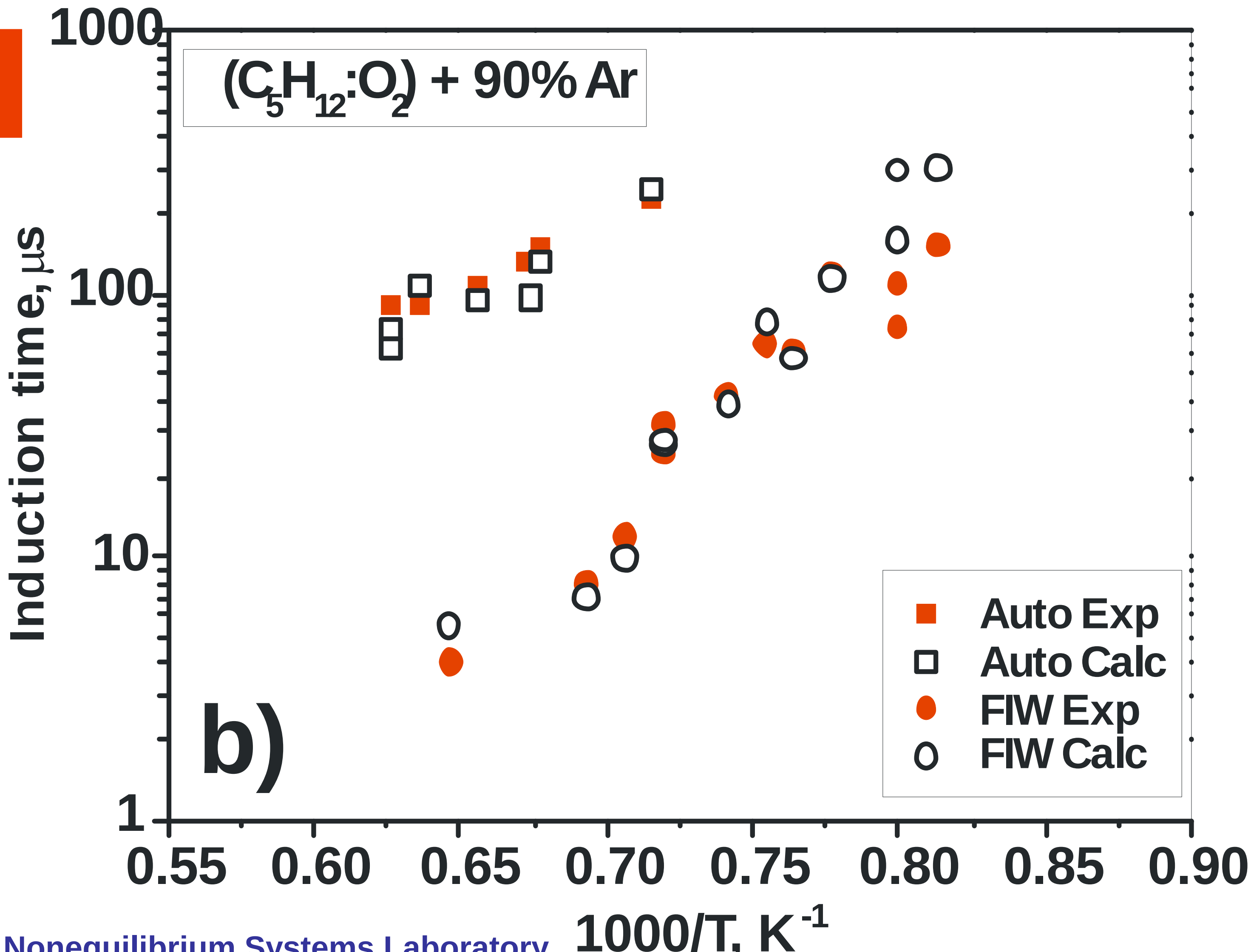


Ignition Delay Time: Methane-Containing Mixture

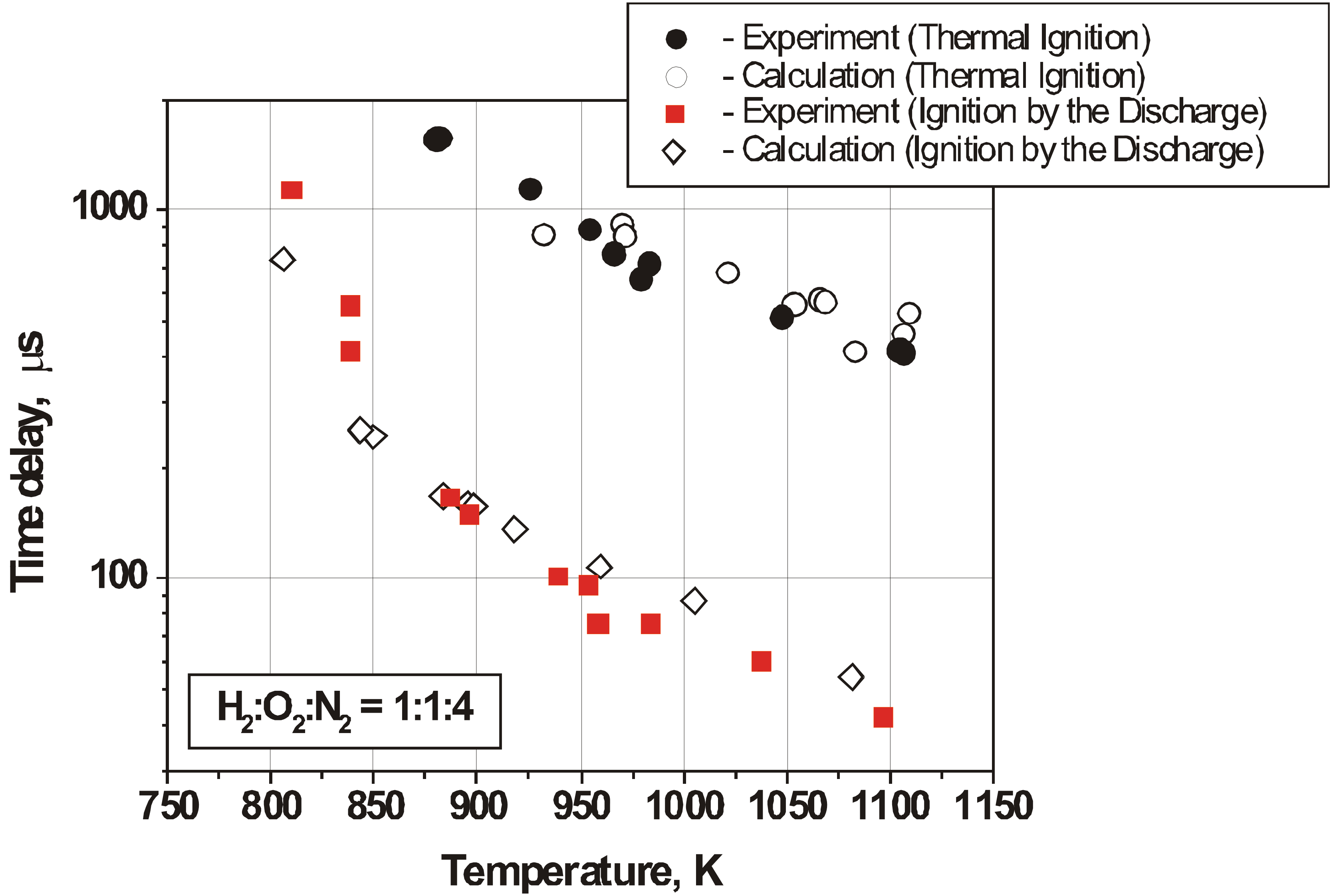


RAMEC (for C1) + Westbrook (C2-C7) + High Pressure Adjustment

C_5H_{12}

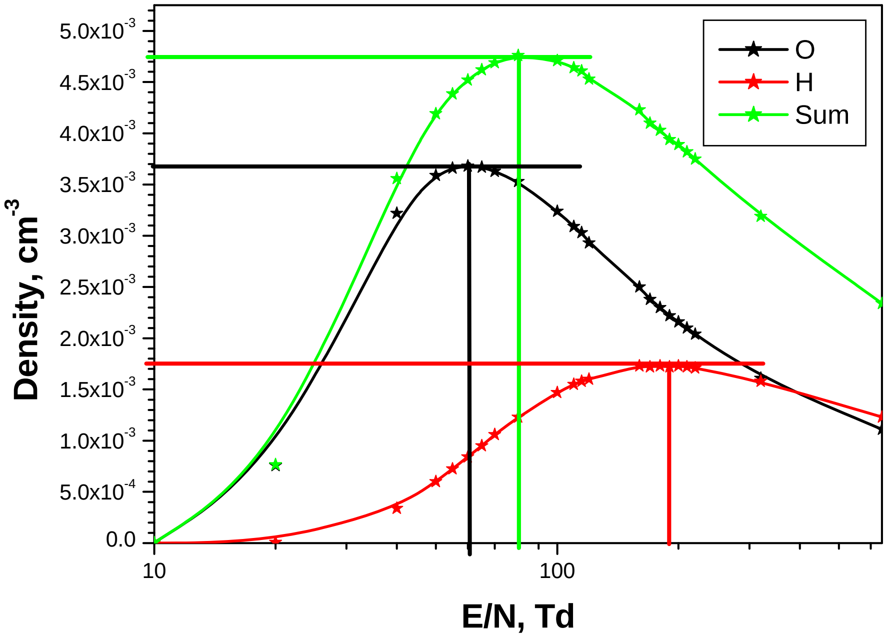


Experiment and Calculations in H_2-Air Mixture

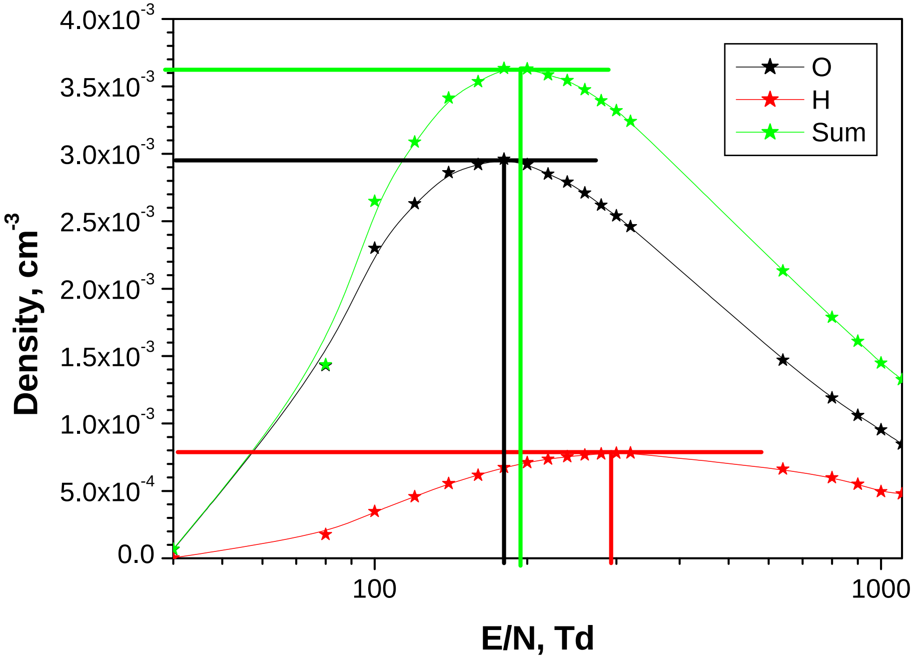


Modeling of Radicals Formation vs E/n ($W=14\ mJ/cm^3$)

H2:O2:Ar=29.5:14.75:55.75

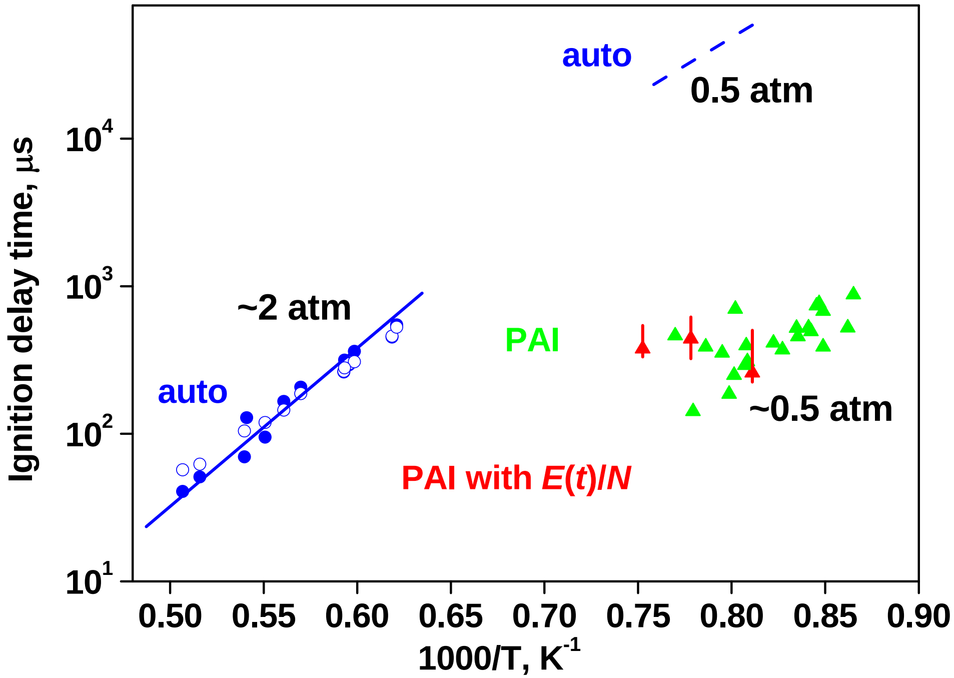


H2:O2:N2=29.5:14.75:55.75

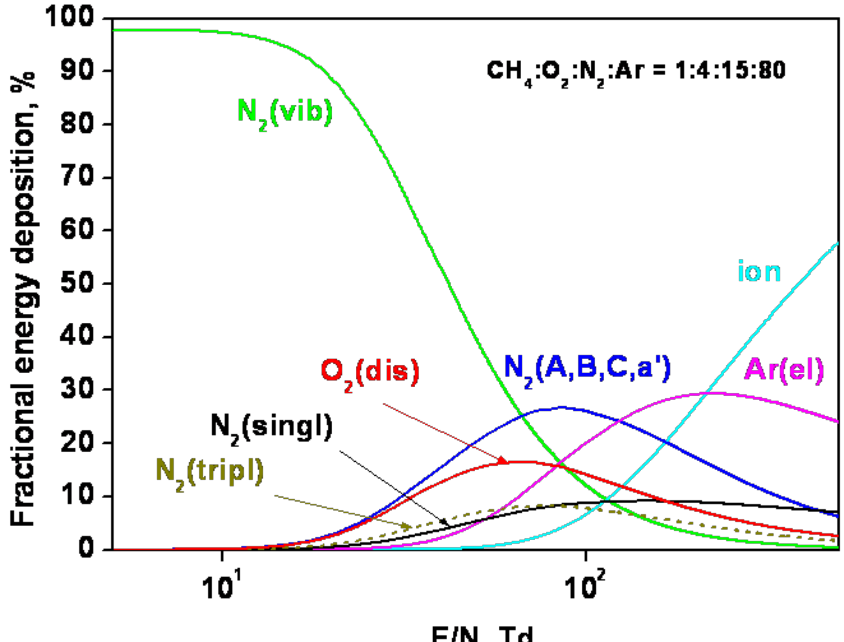


Delay time for autoignition and plasma assisted ignition in CH_4-containing mixture

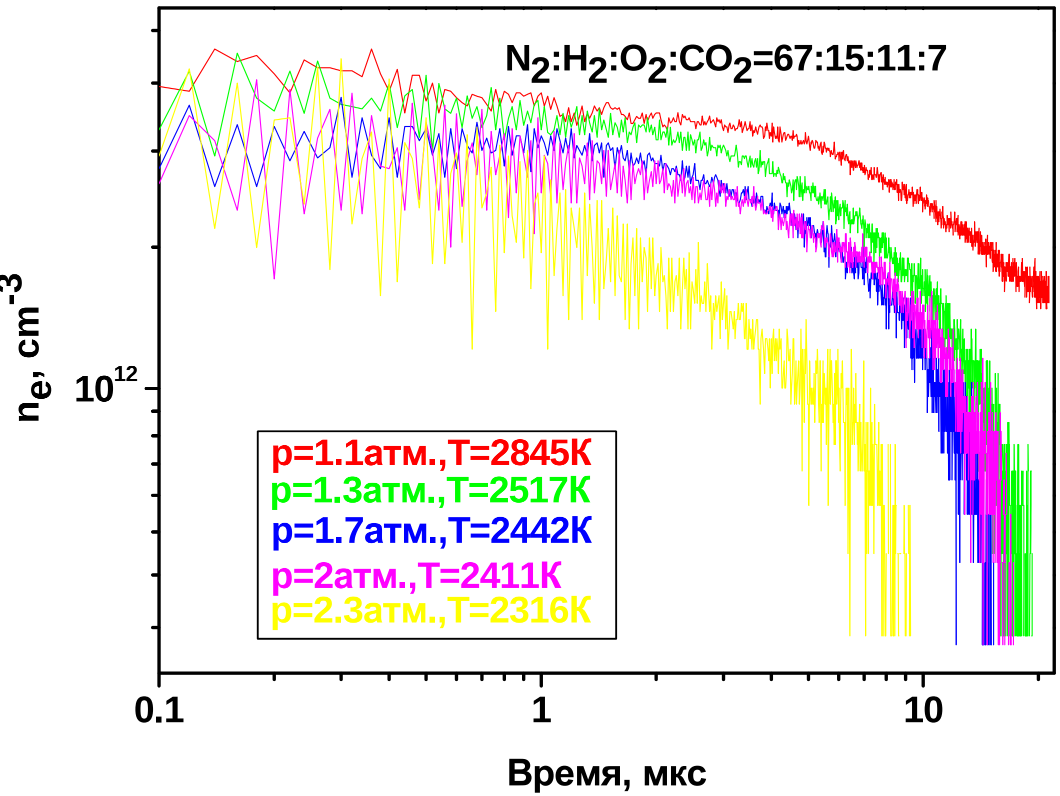
Aleksandrov et al. (2009)

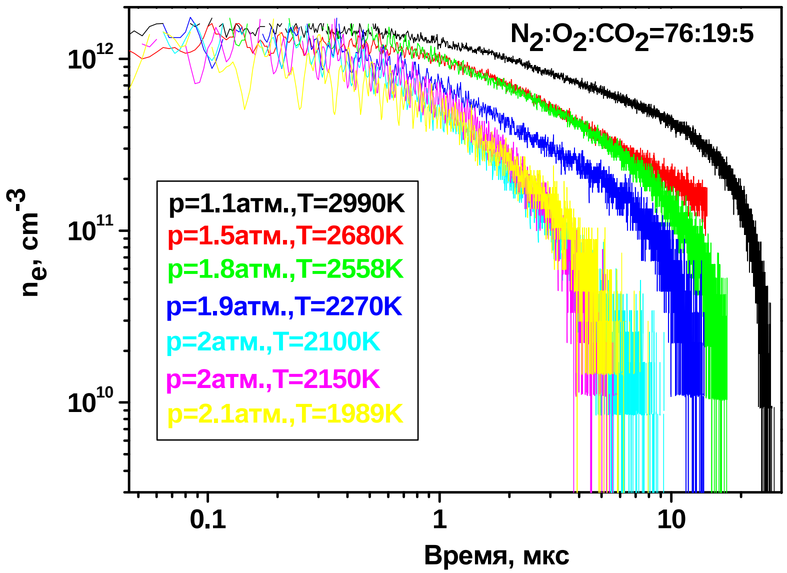


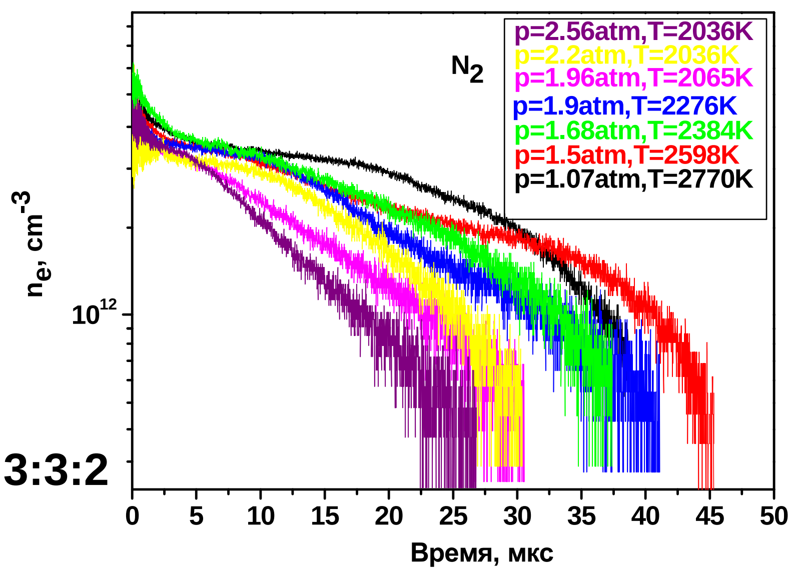
$$CH_4:O_2:N_2:Ar = 1:4:15:80$$



Plasma Recombination at High Pressures and Temperatures





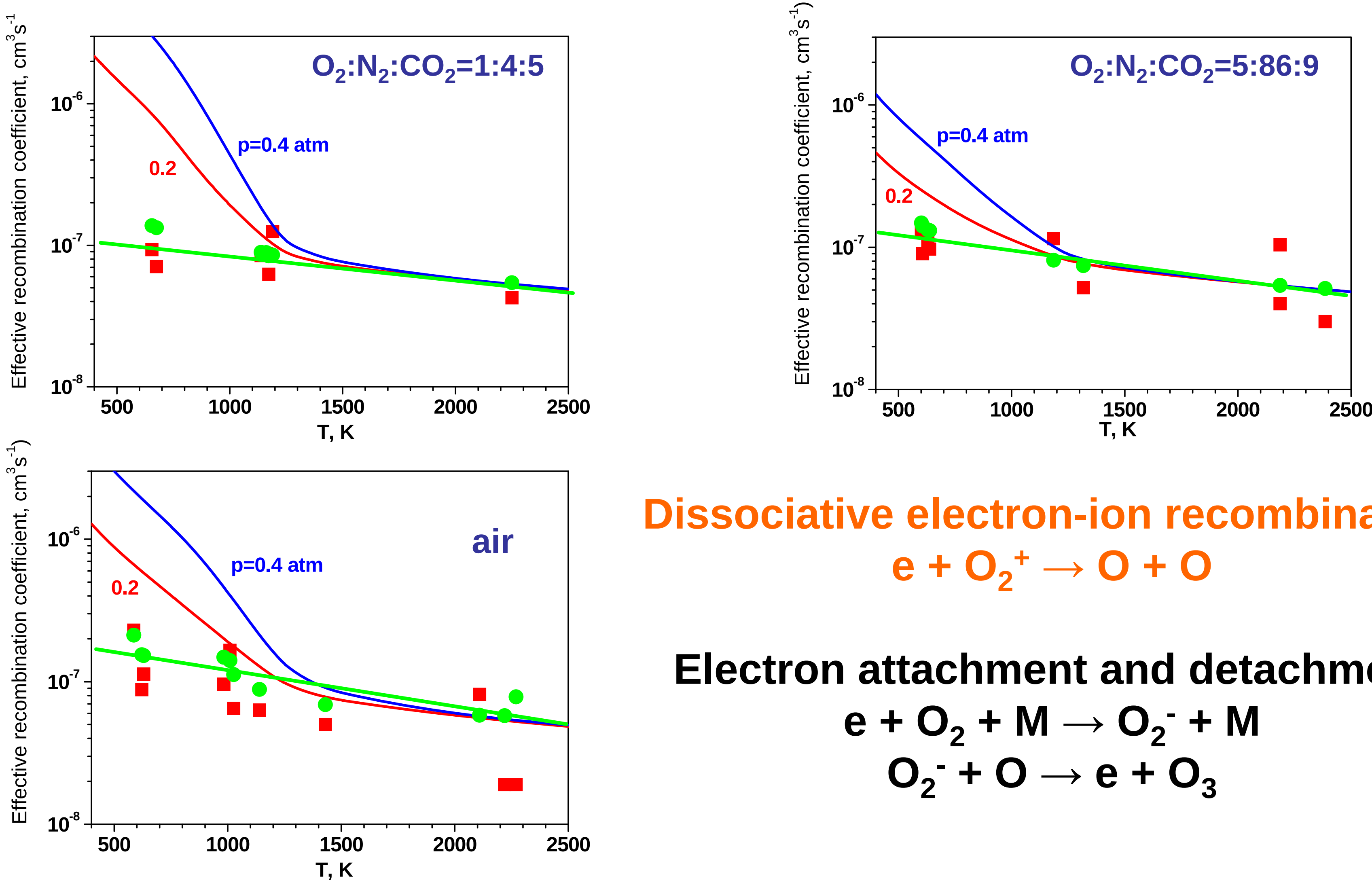


N2:H2:O2:CO2=67:15:11:7

After 10 μs, at 1atm., 2800K

$N_2:H_2O:O_2:OH:CO:CO_2:H:O:H_2$=67:10:5:4:3.5:3:3:3:2

Evolution in Time of Electron Density During Plasma Decay



Dissociative electron-ion recombination

$$e + O_2^+ \rightarrow O + O$$

Electron attachment and detachment

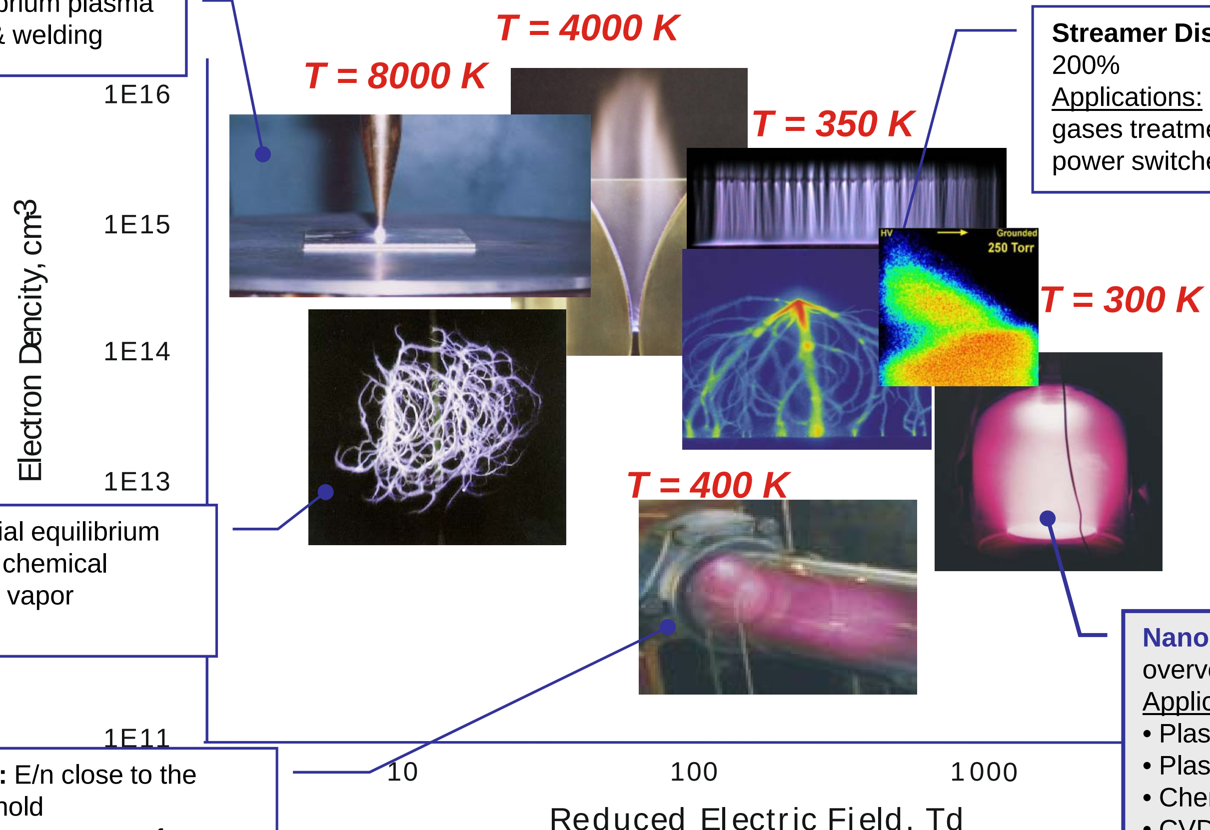
$$e + O_2 + M \rightarrow O_2^- + M$$

$$O_2^- + O \rightarrow e + O_3$$

Types of Gas Discharges and Their Applications

Arc Discharge: equilibrium plasma
Applications: melting & welding

Streamer Discharge: overvoltage up to 200%
Applications: surface treatment, flue gases treatment, electrical breakdown, power switches



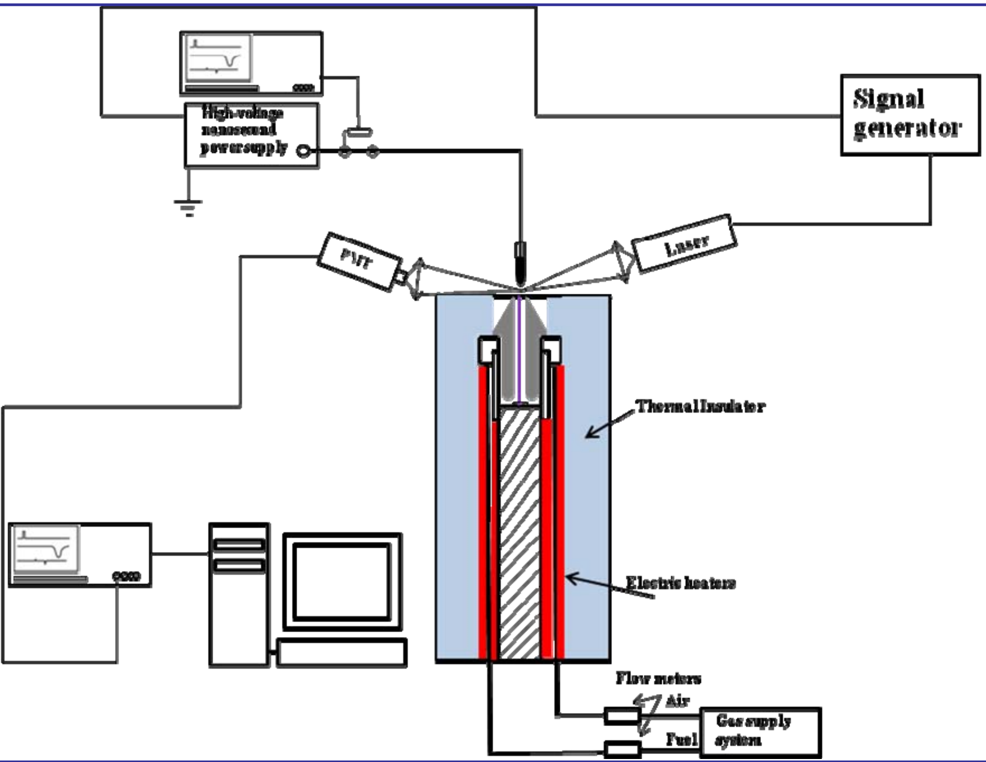
MW Discharge: partial equilibrium
Applications: plasma chemical conversion, chemical vapor deposition (CVD)

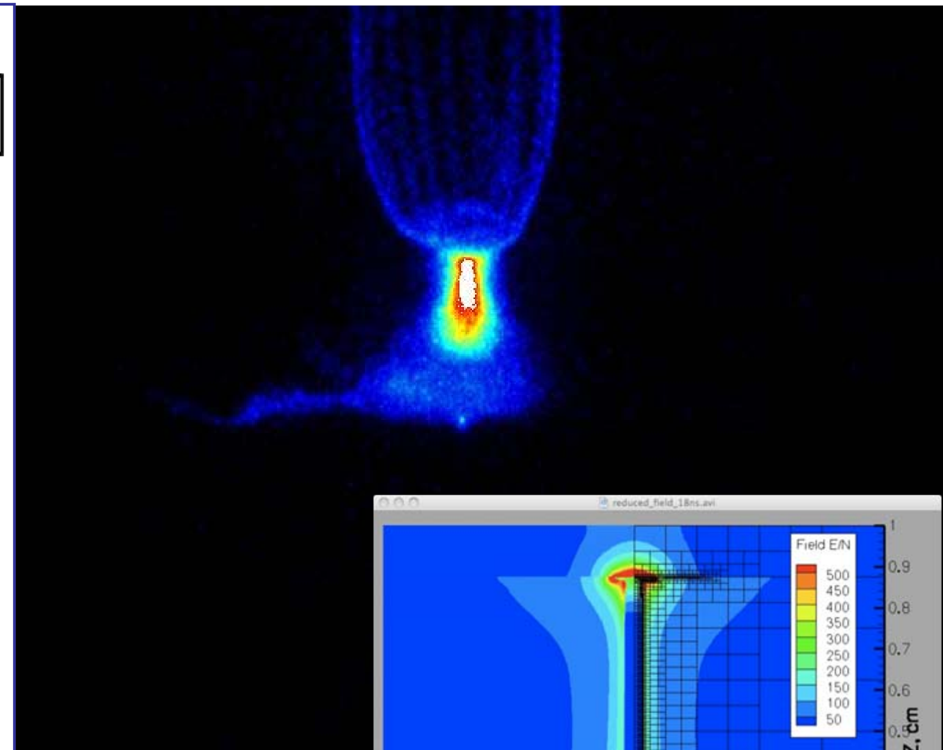
Nanosecond Pulsed Discharge:
overvoltage up to 10 times
Applications:
- Plasma supported combustion
- Plasma supported aerodynamics
- Chemical conversion
- CVD

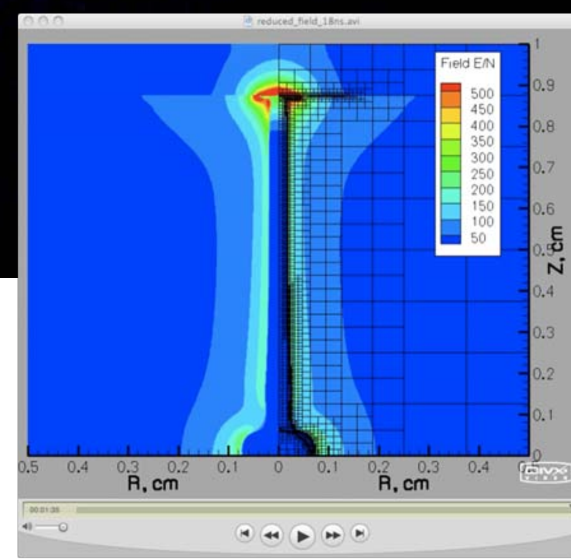
Glow Discharge: E/n close to the breakdown threshold
Applications: light sources, surface treatment, CVD

Discharge Development at Different Overvoltage and Plasma Generation

Setup for OH Dynamic Measurements in Streamer Channel Afterglow





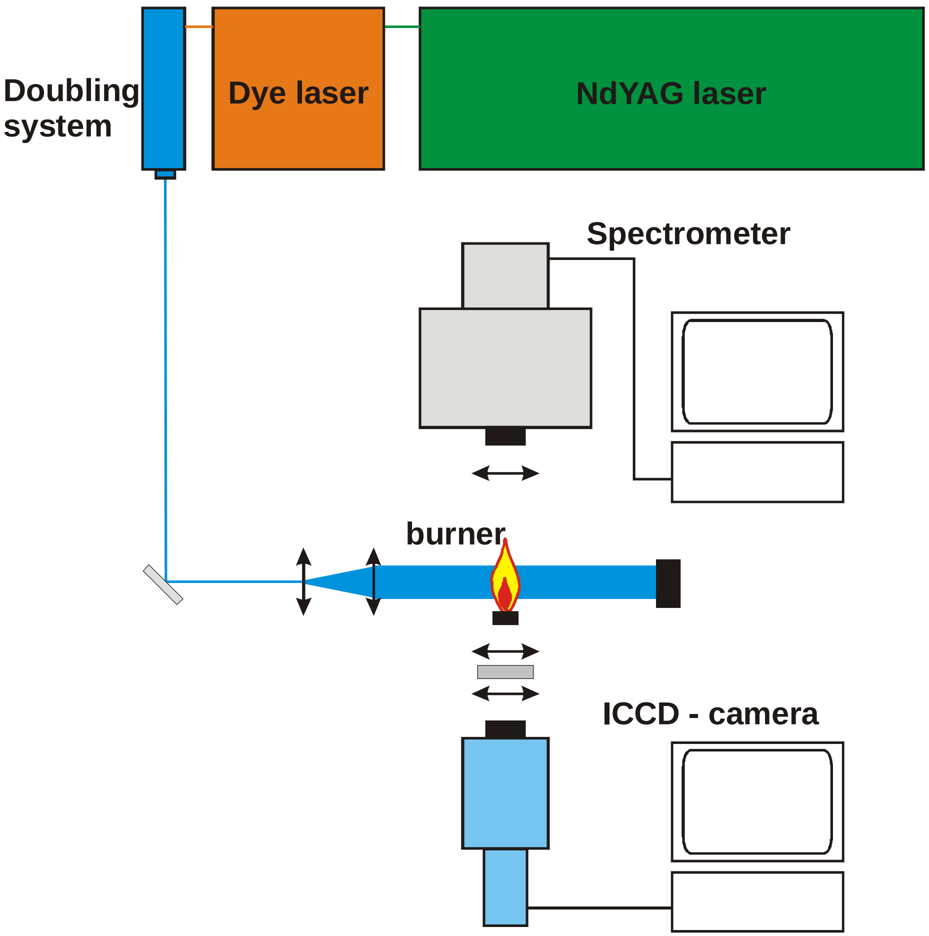


Pancheshnyi et al

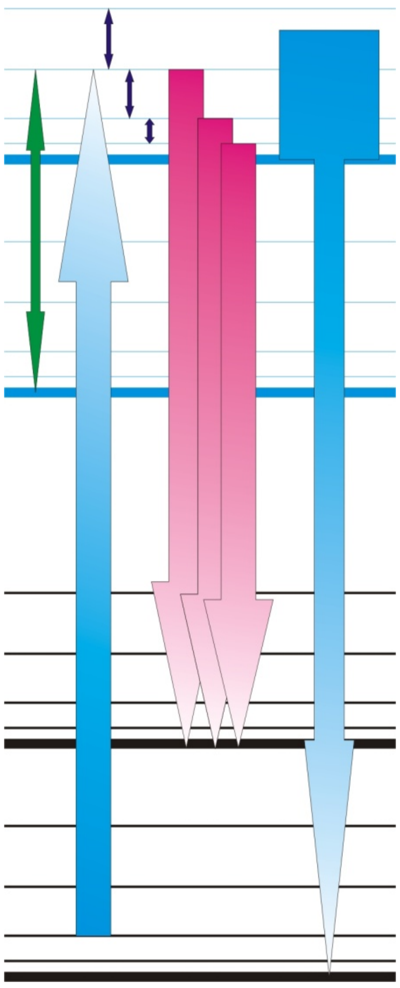
Physics of Nonequilibrium Systems Laboratory

LIF Diagnostics Setup: OH Profile Control

LIF OH



LIF OH



OH (X-A):

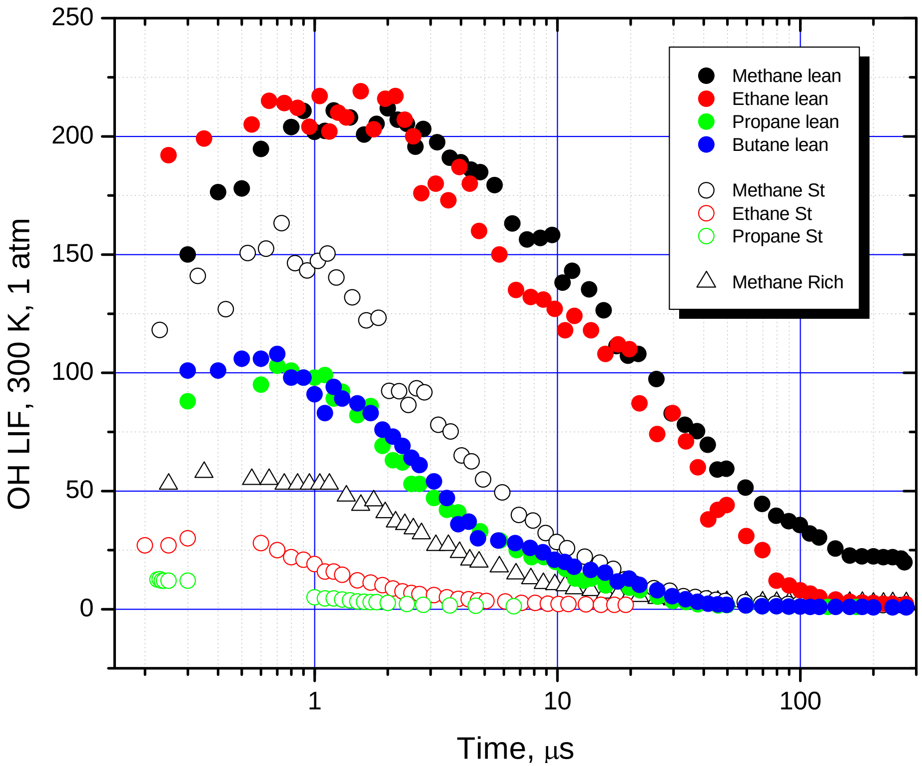
Excitation: $Q_1(6)$ 282.92 nm;

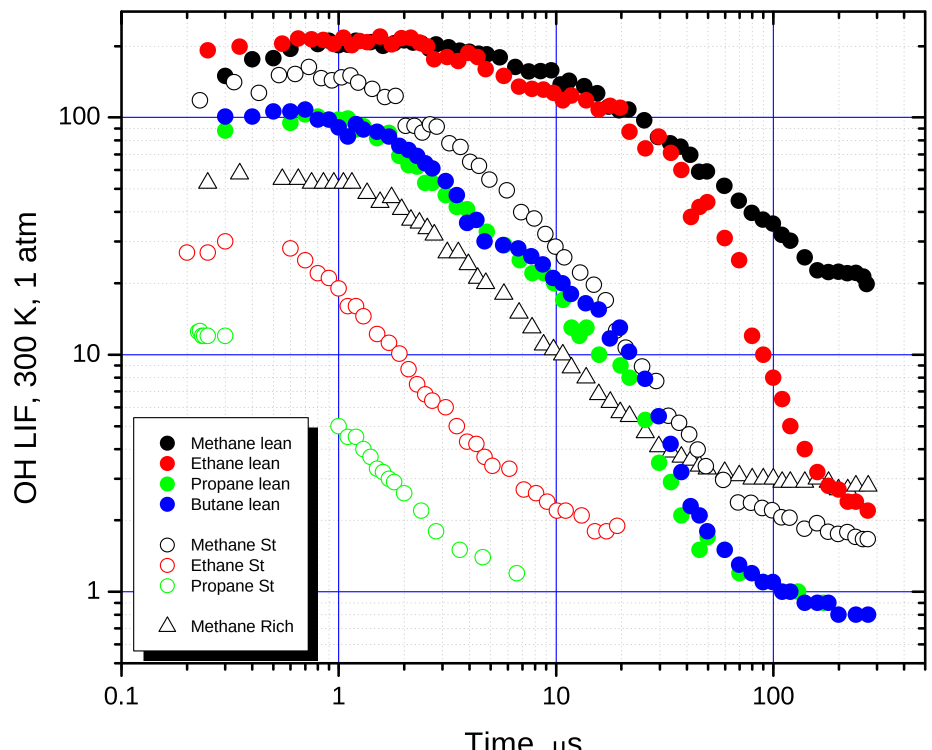
Emission:

315nm, $\delta\lambda$=1.8 нм;

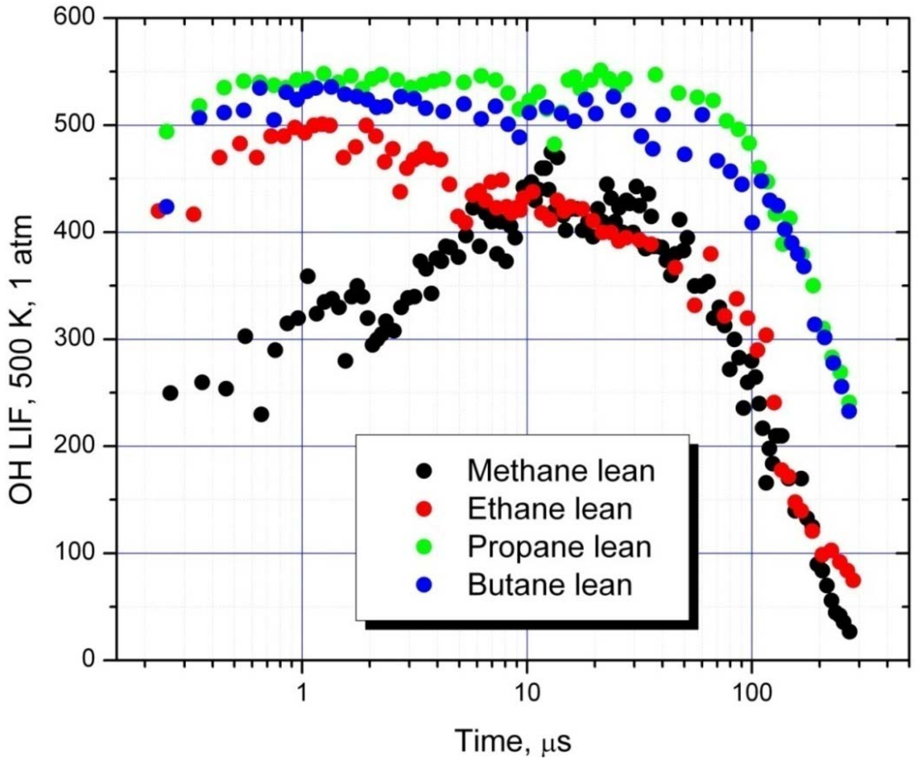
Registration – PicoStar LaVision ICCD камера

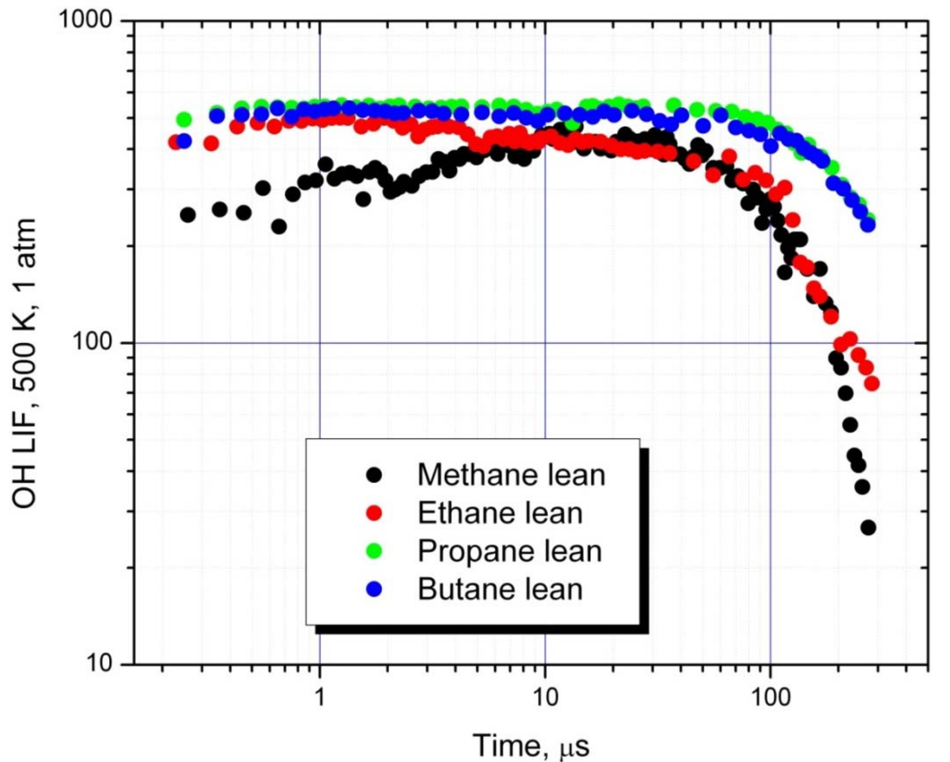
LIF Emission of OH at 300 K



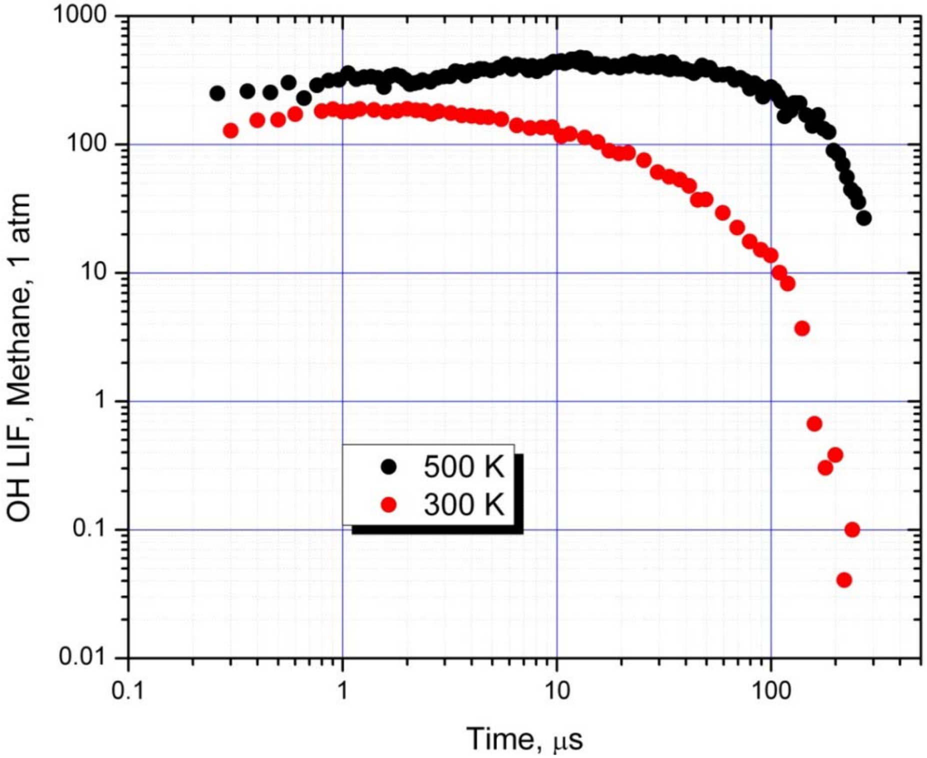


LIF Emission of OH at 500 K

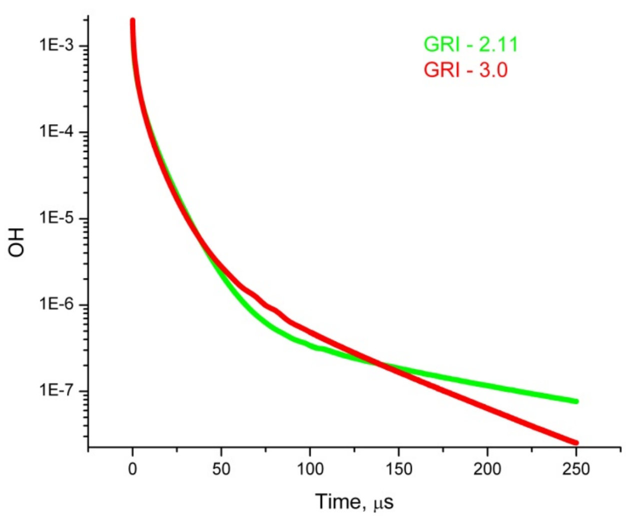




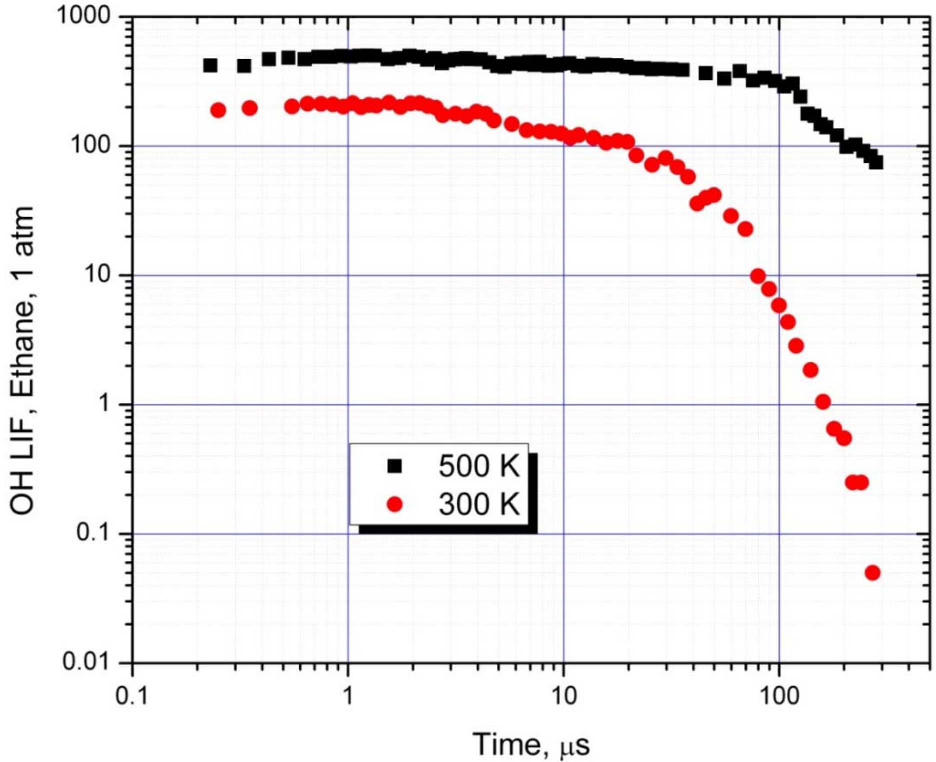
300 K Versus 500 K LIF of OH



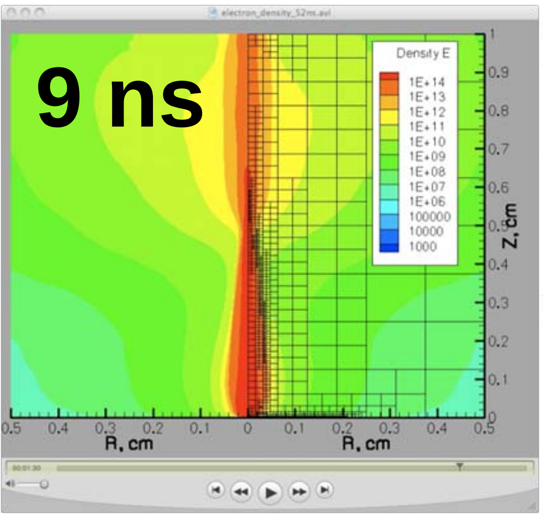
Methane

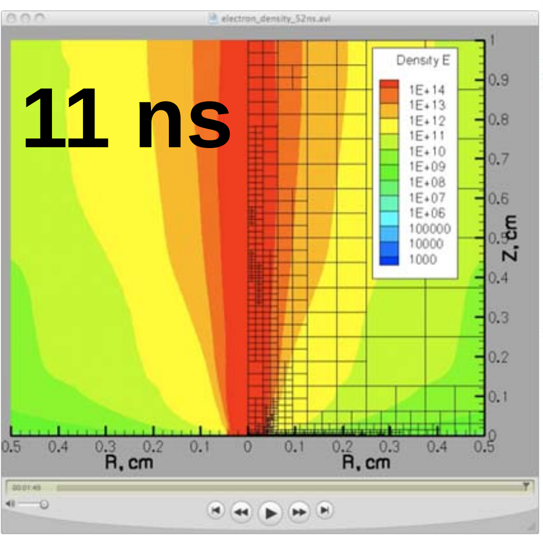


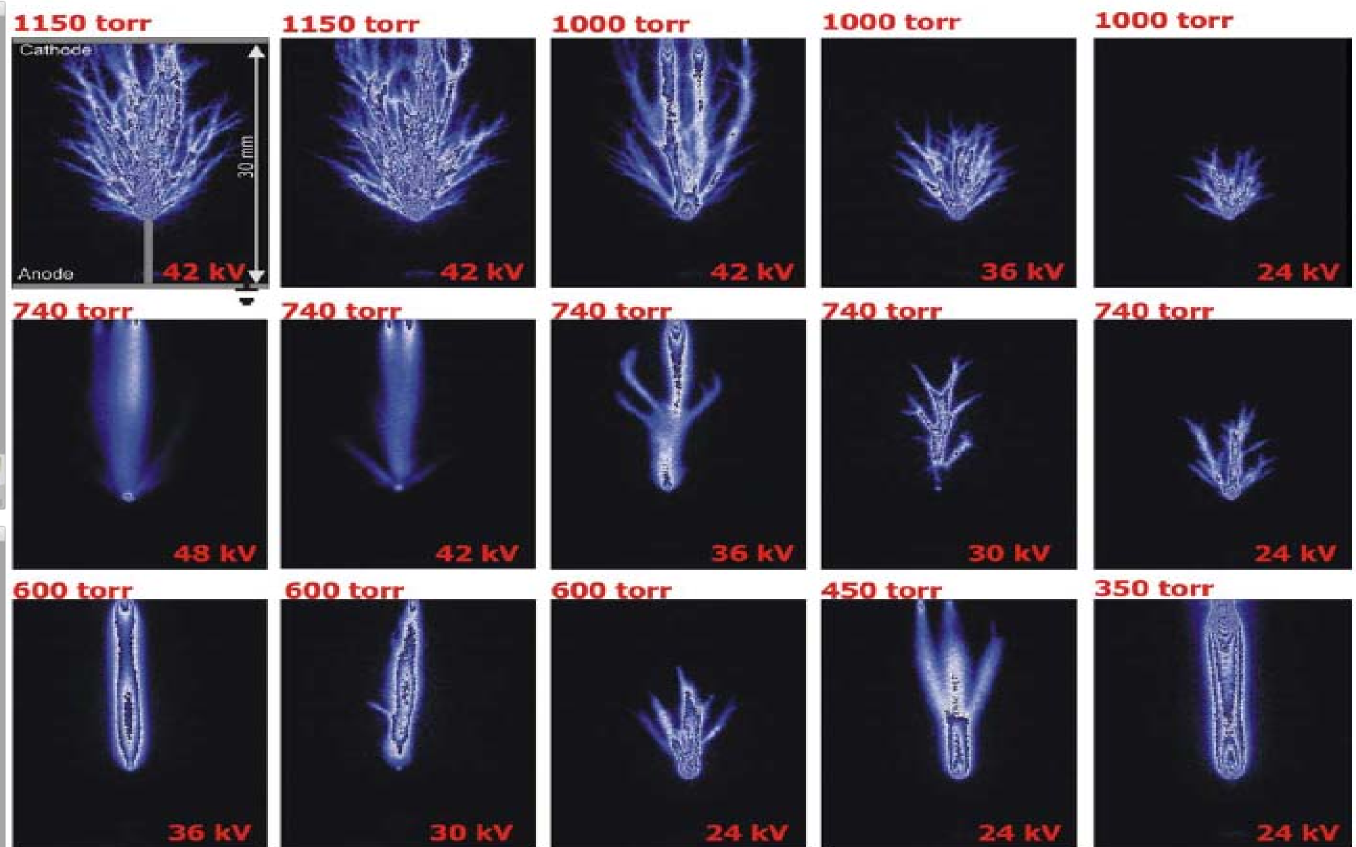
Ethane



High-pressure Conditions: Always Non-Uniform

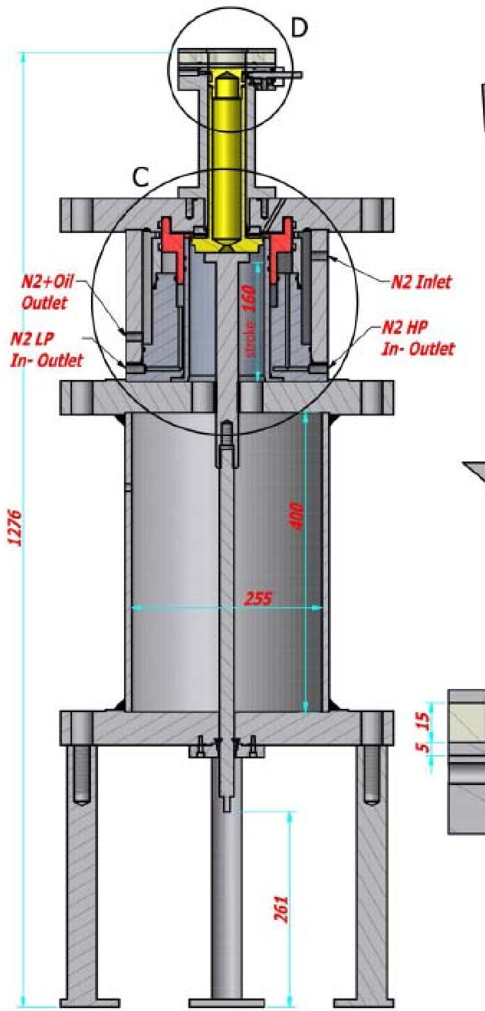


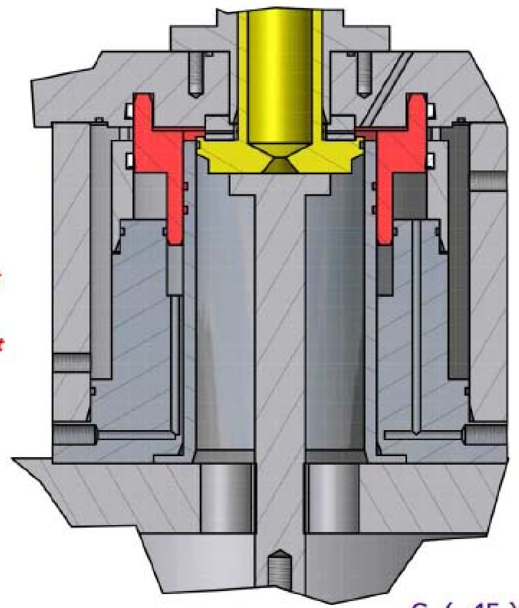


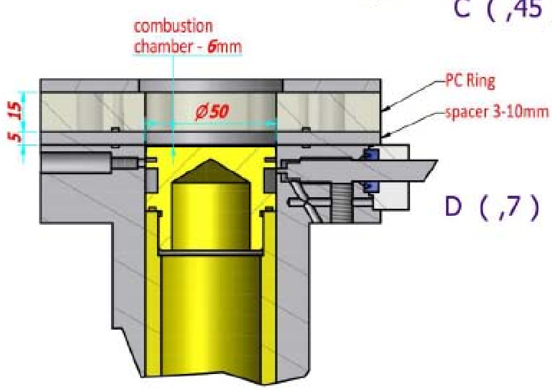


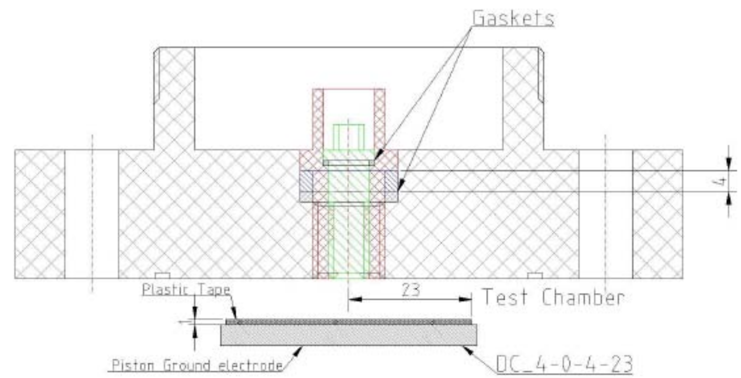
Pancheshnyi et al

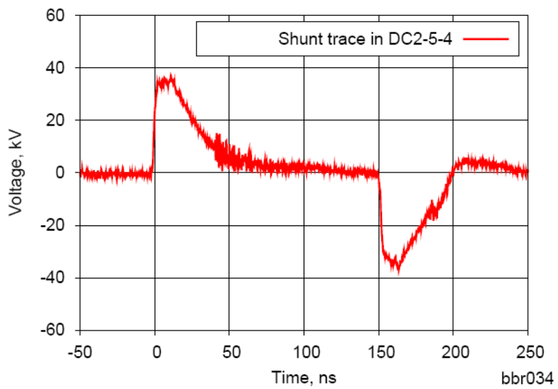
Rapid Compression Machine: High-Pressure, Low-Temperature

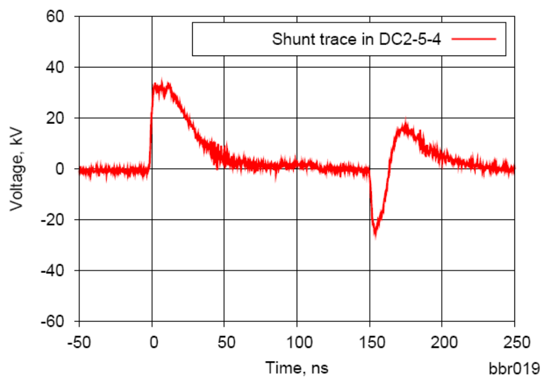




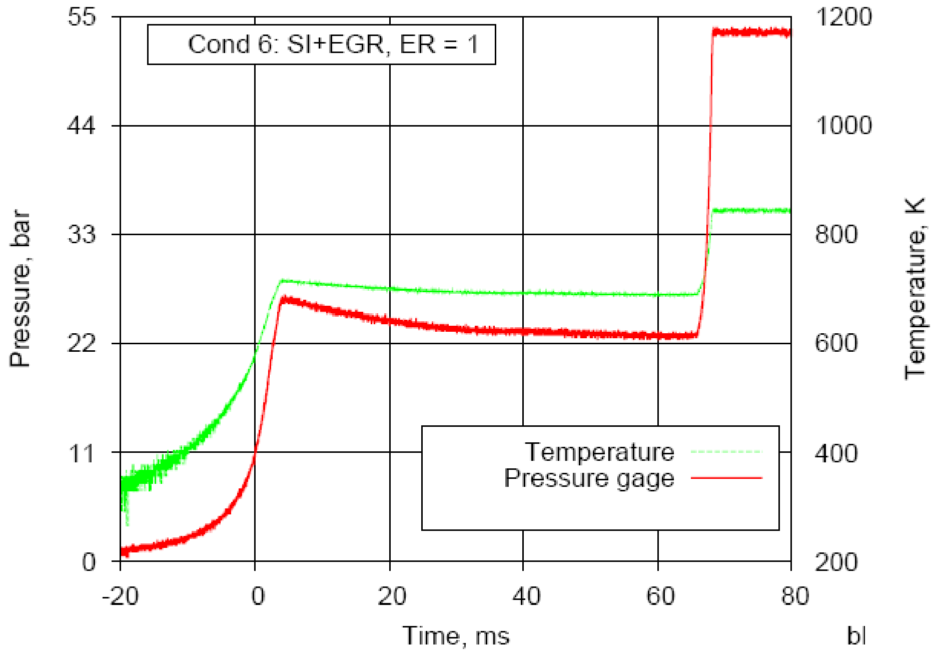




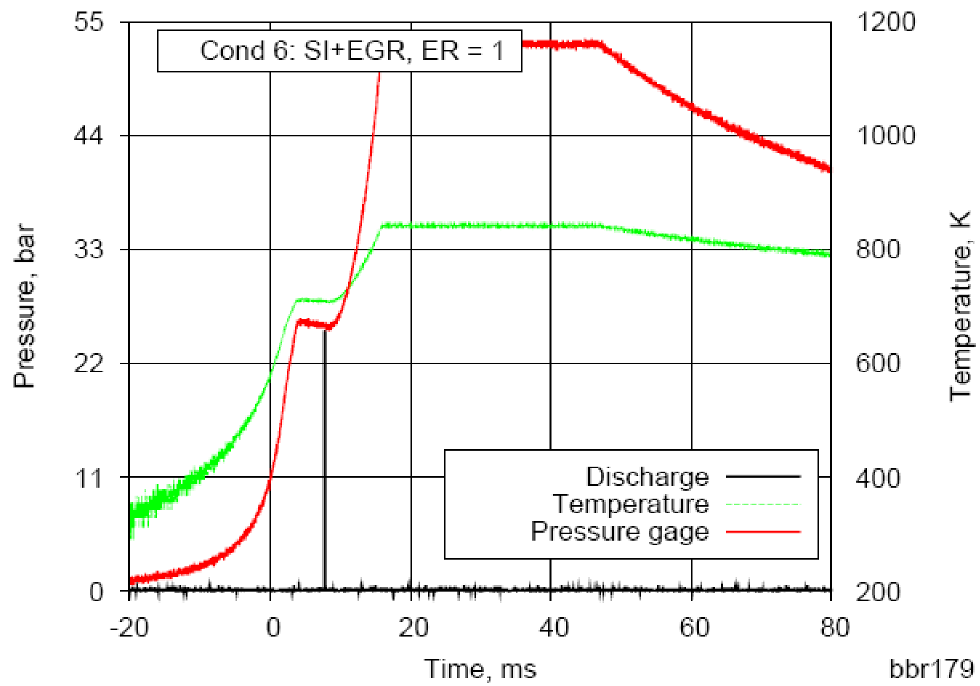




PAC at High Pressure: ER = 1 (Rakitin et al)

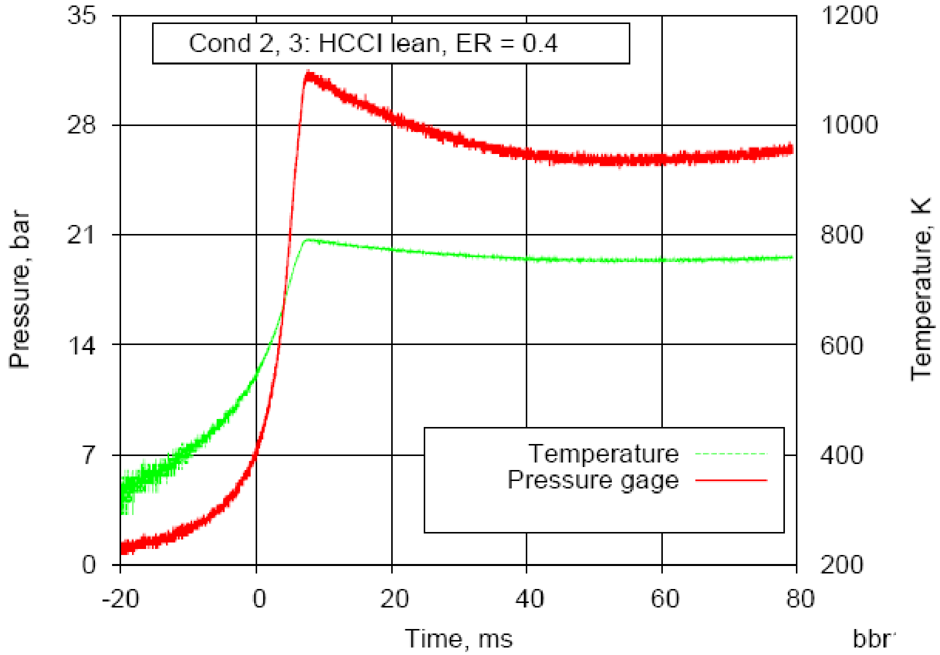


T2 = 713 K
P2 = 26.5 bar



Propane, Surface DBD, < 50mJ

PAC at High Pressure: ER = 0.4 (Rakitin et al)



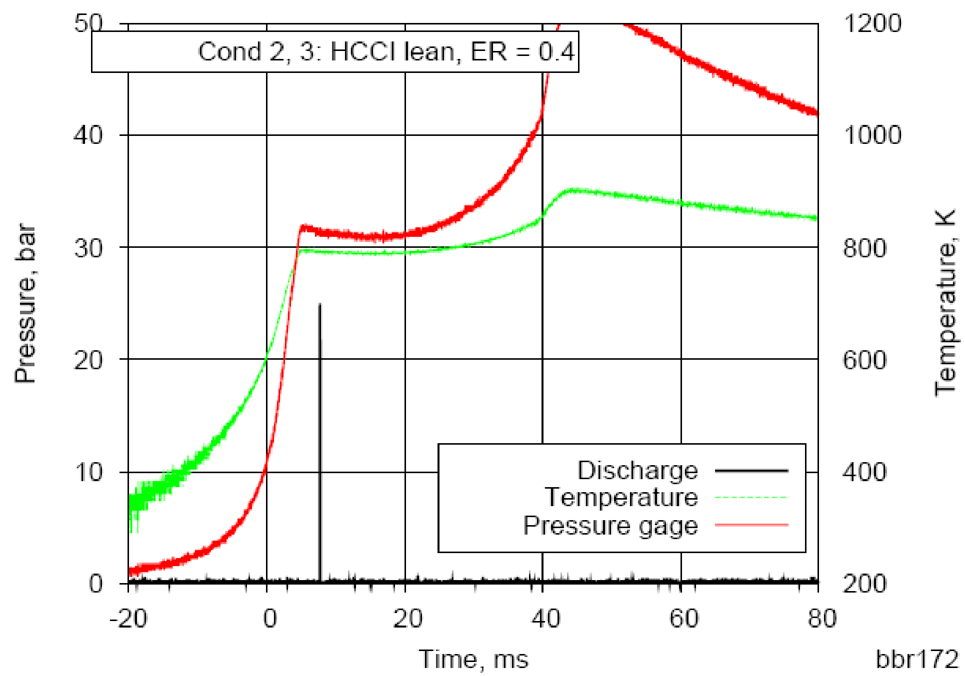
T2 = 794 K

P2 = 32 bar

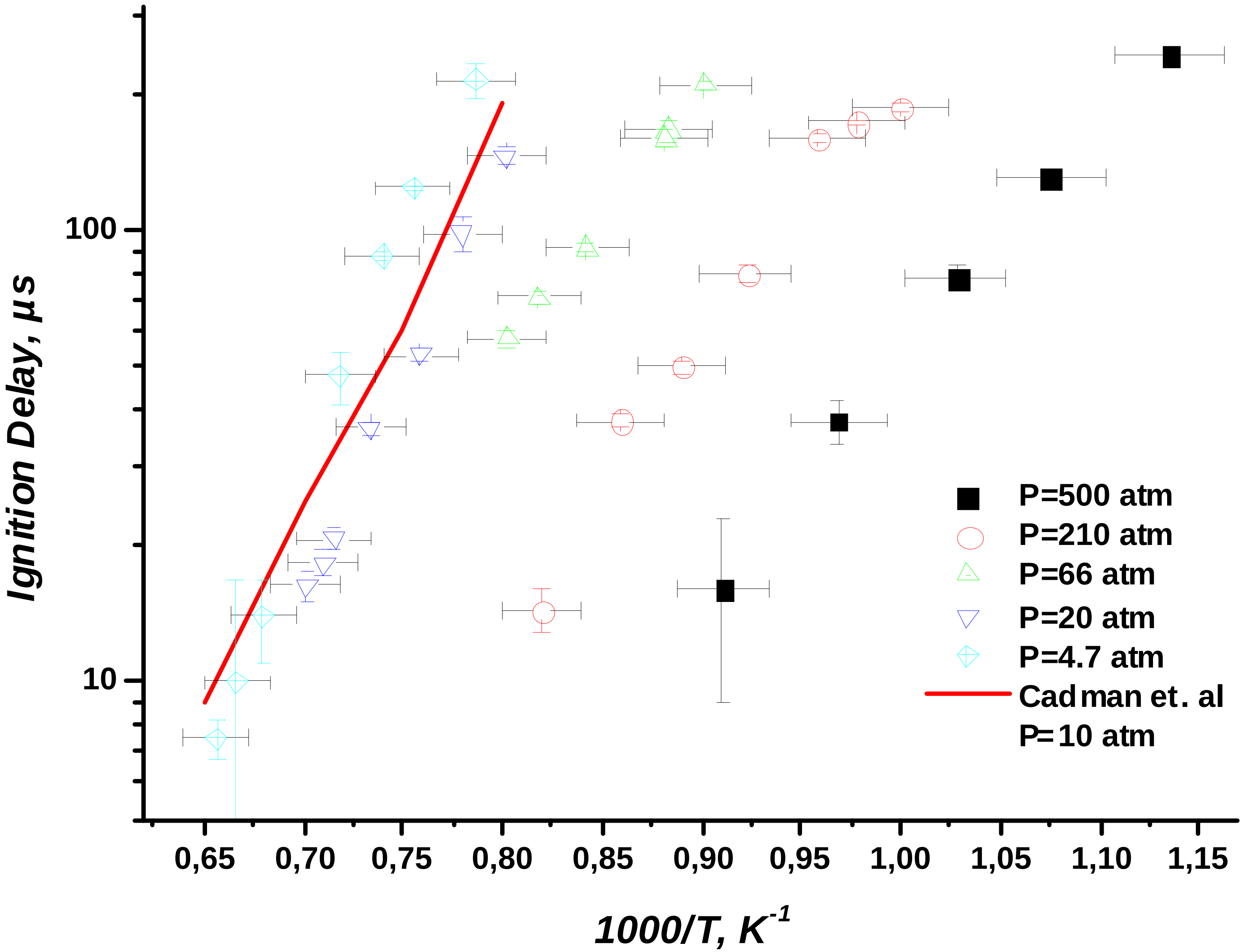
Propane,

Surface DBD,

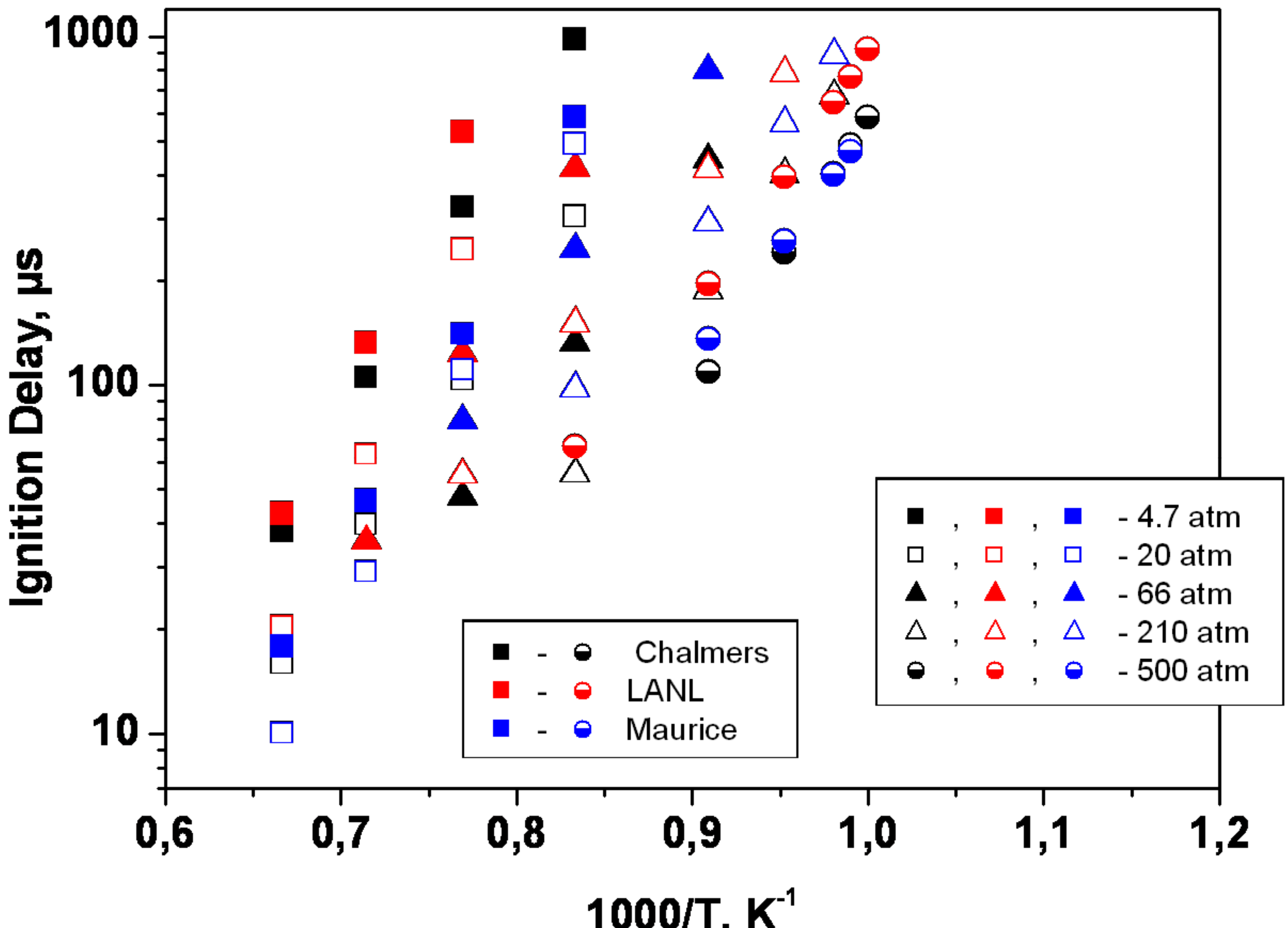
< 50mJ



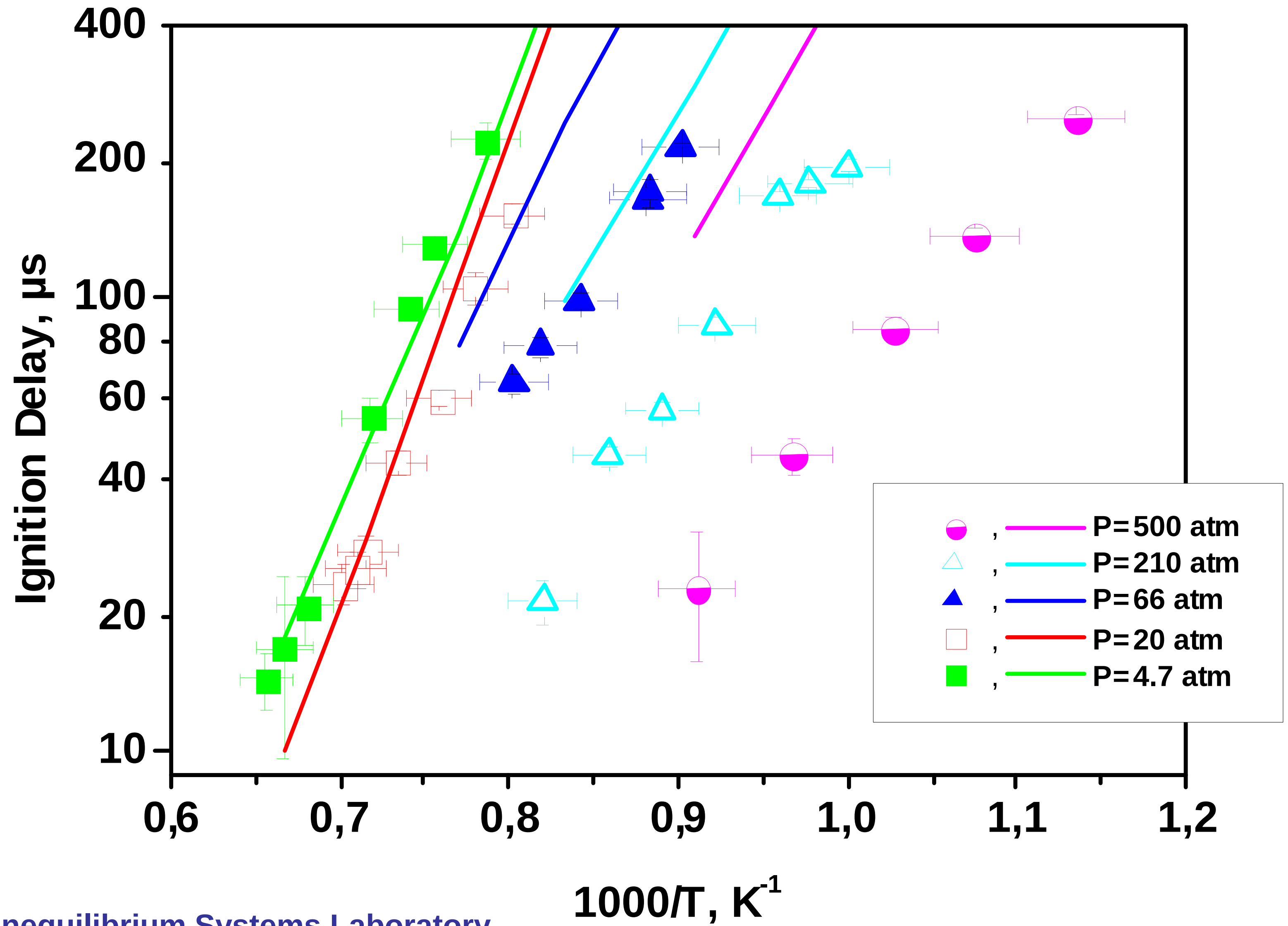
Propane-Butane-Air Lean Mixtures.
$\varphi = 0.5$ (C_3:C_4=85:15)



Propane-Butane-Air Mixture Ignition. φ = 0.5 (C_3:C_4=85:15). Calculations



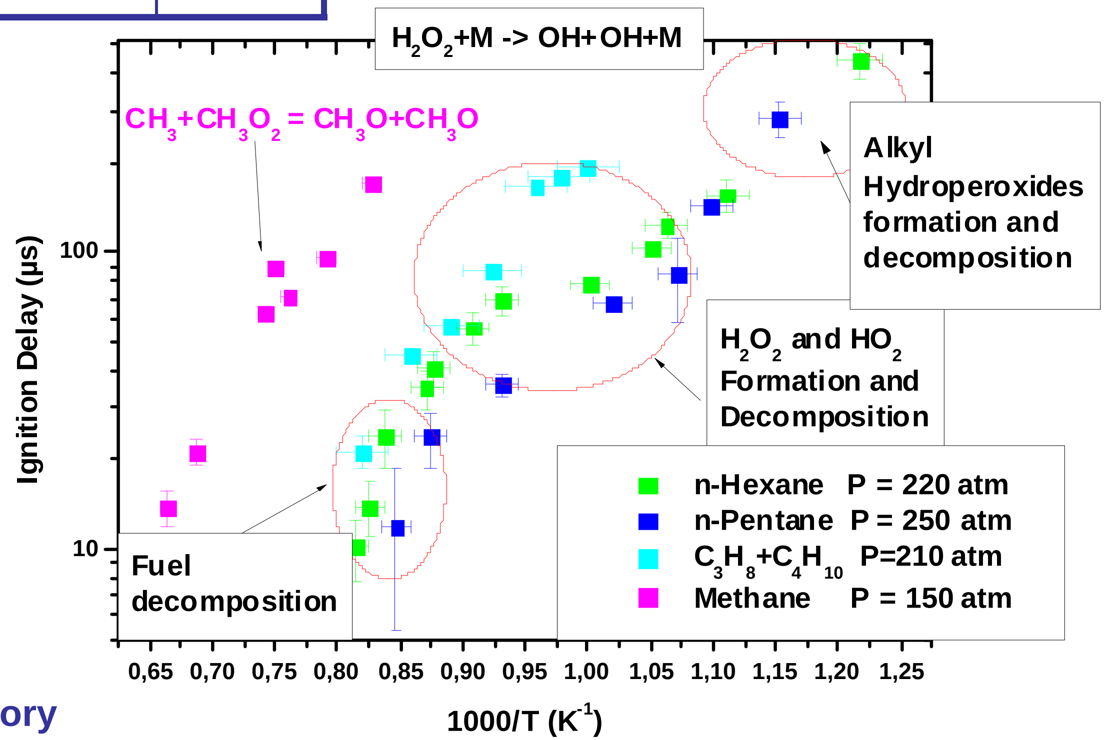
Propane-Butane-Air Mixture Ignition. Experiment vs Calculations.



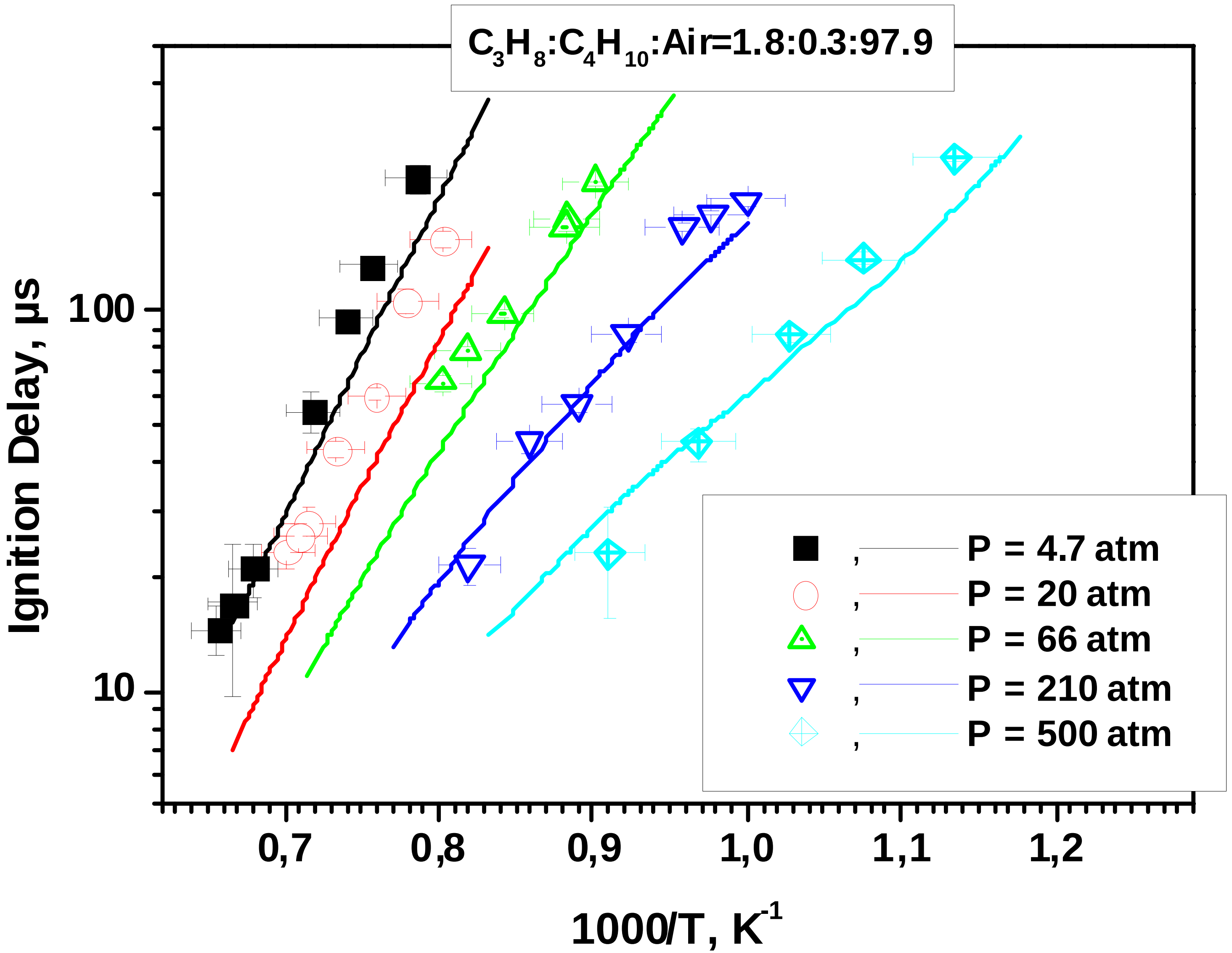
Channels of Kinetic Scheme Optimization

Reaction	T	k
$C_3H_8 + HO_2 = C`H_2C_2H_5 + H_2O_2$	1200	2.5
$C_3H_8 + HO_2 = CH_3C`HCH_3 + H_2O_2$	1200	2.5
$O_2C_3H_7 = HOOCH_2C`HCH_3$	800-1000	0.2
$CH_3CHO_2CH_3 = CH_3CH(OOH)C`H_2$	800-1000	0.2
$OCHCH(OOH)CH_3 = CH_3CHO + HCO + OH$	800	0.2
$OCHCH_2CH(OOH)_2 = CH_2O + CH_2CHO + OH$	800	0.2
$CH_3COCH_2(OOH) = CH_2O + CH_3CO + OH$	800	0.2

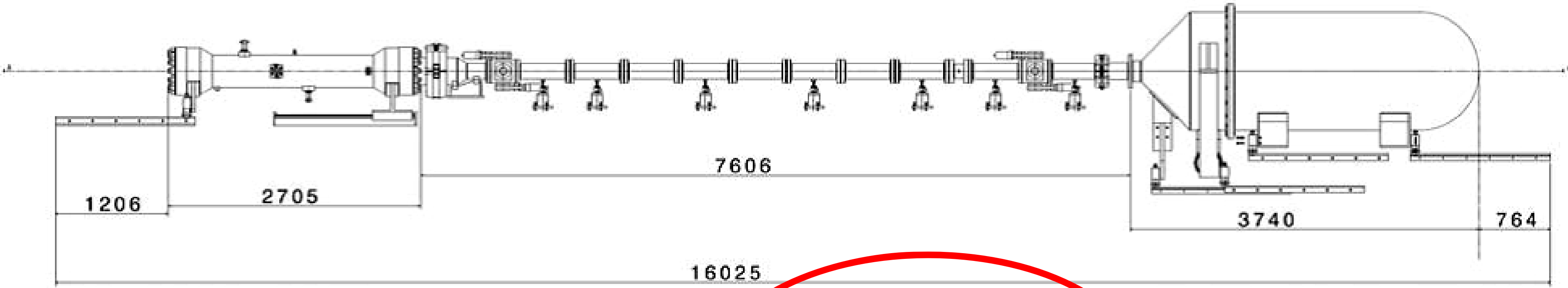
Konnov, Potapkin

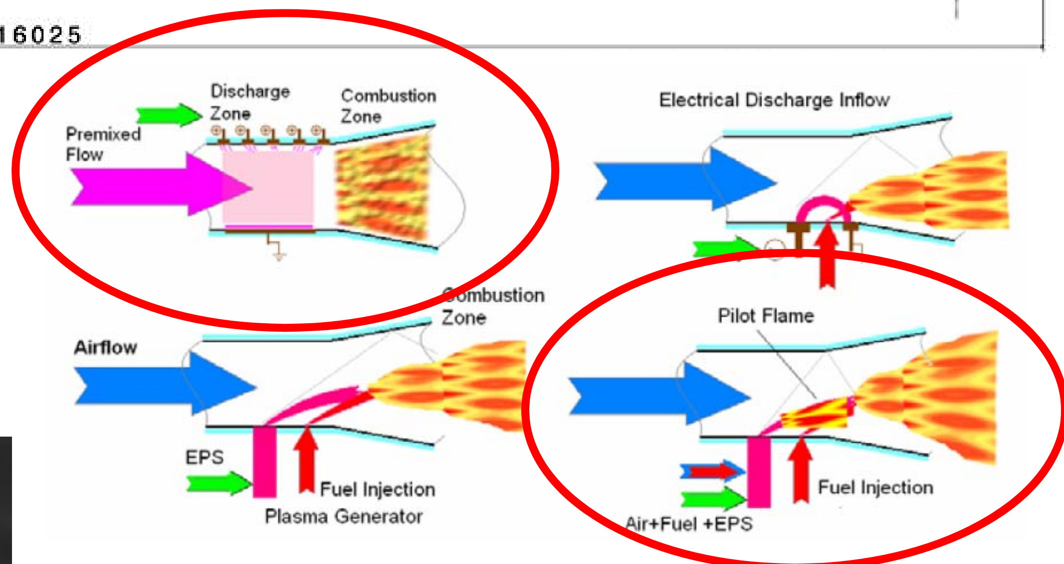


Mixture $C_3H_8:C_4H_{10}:Air = 1.8:0.3:97.9$



Discharge Formation and Flame Stabilization in High Speed Flow





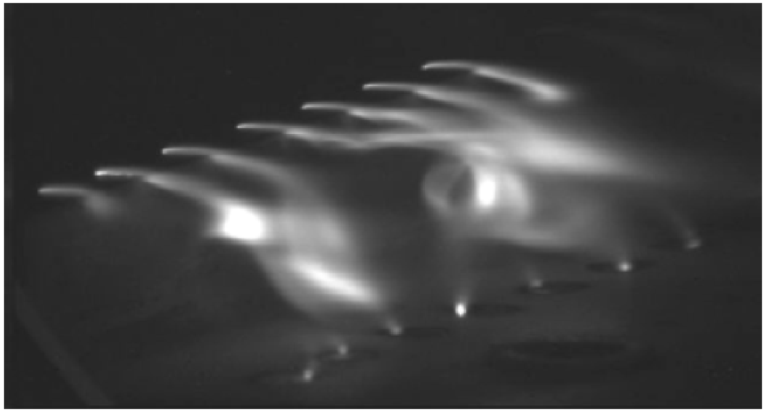
IVTAN (Sergey Leonov):

M = 2

Maximal stagnation pressure 1.8 Bar

Stagnation temperature 670 K

Discharge Power ~ 1 kW



DPI Shock Tunnel:

M = 2-5

Static pressure 0.1 - 1 Bar

Static temperature 700-1000 K

Discharge Power ~ 1 kW

Summary

Experiment:

Shock Tube
Shock Tunnel
Rapid Compression Machine
Premixed Flow Nozzle

Range of Parameters

P = 0.1 – 70 atm
T = 300 – 2000 K
M = 0 - 5
ϕ = 0.01 – 1
E/n = 200-500 Td (Air)
Fuels: H_2, C_1 – C_4
Acetones, Alcohols, CO

Theory:

Discharge Models
Plasma Models
Chemical Kinetic Models